SUMMARY REPORT OF THE SUMMER CONFERENCE

DARPA-MATERIALS RESEARCH COUNCIL

La Jolla, California

July 1989

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The University of Michigan
Department of Chemical Engineering

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of the

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INTRODUCTION

This report is a summary of the 1989 DARPA-Materials Research Council Summer Conference which was held in La Jolla, California, during the period from July 10, 1989 through August 4, 1989. It is a report which is being submitted to DARPA early in the contract period to enable them to utilize the results of the various workshops in a timely fashion. A later report will be issued to include the materials generated at workshops held at periods other than those of the Summer Conference.

The principal task of the ONR-DARPA Grant is to bring together a group of the Country's leading materials scientists and engineers for an extended period, usually the month of July, to permit them to apply their combined talents to the planning and scoping of future materials research areas for the Department of Defense.

During the year workshops, and in some cases program reviews, are attended by smaller groups of Council members and their reports are made directly to DARPA. This is a growing activity of the Council and these reports in the future will be included in the report submitted at the end of the contract year.

The technical direction of the Council is by a Steering Committee made up of five representative members of the Council who work with DARPA management. The Committee for 1989 is given in the following table. The Steering Committee selects the relevant topics for the annual Summer Conference and works with the other council members in developing new areas in materials research. The membership on the Steering Committee and of the Council varies from year to year depending on the research areas that are of major interest to the Department of Defense. The Council membership for 1989 is given in the following table.

The Council also serves as a resource for the DARPA Defense Sciences Divisions and other DARPA offices. The DARPA participants in the 1989 Summer Conference are given in the following listing.

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Dr. Louis Auslander DARPA-MSD	Dr. Richard A. Reynolds DARPA-DSO	Dr. Ben Wilcox DARPA-MSD
Dr. W. Barker DARPA-MSD	Dr. Kay Adams DARPA-MSD	Dr. Andrew C. Yang DARPA-ESD
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Dr. Frank Patten DARPA-MSD	Dr. Ira Skurnick DARPA-ESD	

The agenda for the Summer Conference is prepared initially during the prior year's conference with input from DARPA and the Council. This is refined at subsequent Steering Committee meetings and the workshops are organized. The calendar for the 1989 Summer Conference is shown in the attached figure.

JULY 1989 SUMMER CONFERENCE

(Conference dates are July 10th through August 4th)

TORREY PINES ELEMENTARY SCHOOL
8350 CLIFFRIDGE AVENUE
LA JOLLA, CA 92037

S	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY	S
	10 DARPA - MRC DAY	11 ← MANUFACTURING SCIENCE AND MATHEMATICAL MODELING & SIMULATION →	12	13	14 DESIGNING WITH ADVANCED MATERIALS	
	17 INTERATOMIC POTENTIALS Ste. Cte. Meeting	18 REFRACTORY COMPOUNDS NOVEL DEVICES	19 ← LIMITATIONS ON FUTURE VLSI →	20	21 SEMICONDUCTOR PROCESSING AND SENSORS	
	24 DEV. OF NEW PIEZOELECTRIC COMPOSITES BALLOTECHNICS SAIC	25 HIGH ENERGY MATERIALS	26 BIOMIMETRIC DESIGN	27 CRAIG FIELDS ASSIGNMENTS Ste. Cte. (PM)	28	
	31 ← NEURAL NETWORKS AND CELLULAR AUTOMATA →	1	2	3 WRAP-UP	4 Ste. Cte. Meeting	

TABLE OF CONTENTS

TITLE	PAGE

WORKSHOP ON THE FUNDAMENTALS OF MANUFACTURING ADVANCED MATERIALS AND COMPONENTS

H. K. Bowen, R. Mehrabian, J. C. Williams, W. Barker and K. Adams

I. EXECUTIVE SUMMARY

Manufacturing excellence has been recognized as the strategic advantage in the world of industrial competitiveness and productivity[2,8]. It is also the key underpinning for a cost effective and timely defense production system[23]. Current systems upgrades and future DoD requirements will require a strong industrial base; and within that base one of the most vulnerable yet critical areas is the manufacture of advanced materials and components. The MRC was challenged to determine the critical issues in materials manufacturing and to provide specific suggestions for DARPA initiatives to eliminate or alleviate the root causes of deficiencies through the generation of knowledge, understanding and successful demonstration experiments.

Manufacturing in the sense of this paper includes all those intellectual, people and physical processes involved in the development of products and processes, in the actual production of products, and includes aspects of the sales and field service functions. In the modern competitive world, manufacturing can only be examined and understood in a holistic manner. However, the ad hoc nature of manufacturing and the perception, especially in the U.S., that it is not a discipline based practice, presented the workshop organizers with an opportunity to develop both a concept and pathway to resolve the key issues in materials and components manufacturing.

The first step was to determine whether a diverse set of leading industry practitioners could agree that manufacturing may be discipline based as demonstrated by the fact that there were rules for manufacturing. These rules or tenets may be well established or less well accepted. Given that there are rules for advanced materials manufacturing (including a set which need extensive study and verification) and given that new principles may be discovered through appropriate research, then a foundation could be established which would be based on facts and principles to assist in rebuilding our U.S. manufacturing base.

The Workshop was organized for these explicit purposes and working groups were formed to analyze in detail the data accumulated through outside study and most significantly from the invited experts. The consensus from the participants was that there is an incipient manufacturing discipline. For example, there are:

(i) Known rules for manufacturing; such as:

a. Cost is an increasing function of complexity
b. Decreasing variability reduces cost; reducing variability improves performance
c. Technology applications are enhanced after or in conjunction with the implementation of principles of total quality management.
d. Manufacturing excellence is measured by cost, quality, time and flexibility.

(ii) Rules which need further clarification through collection and analysis of available date; such as:

a. Maximizing quality will reduce costs.

b. Minimization of all forms of waste increases quality.

c. Manufacturing competitiveness is independent of volume.

d. Manufacturing excellence is measured by cost, quality, time and flexibility.

(iii) Rules which need substantial research and which are recommended for DARPA initiatives.

It is important to understand that looking at manufacturing as a discipline is a new activity and the most of these rules need quantification and definitions which will only come through the rigorous mindset of traditional engineering research. The ranges of validity, the methods of application, and the empirical relationships and parameters need to be fully understood to create the discipline which will establish manufacturing as a desirable corporate activity and profession and most significantly do what American industry could do so well, be world class manufacturers.

The recommendations for DARPA initiatives are the result of the Workshop and the post-workshop analysis by MRC members:

Establish Methods, Tools and Principles for Process Knowledge and Control

The most significant missing link in our U.S. manufacturing systems is the depth of knowledge about processes, machines and systems to drive the incremental and innovative improvements to meet the new world class metrics of manufacturing performance. The breadth and depth of understanding to be gained is not garnered from "sand box research" but must be obtained in an actual product delivery system. The goal of this initiative is not a particular product or manufacturing system but the knowledge of what to, how to, when to

and with whom to produce world class products --- principles arrived at through the construction and running of demonstration factories. It is proposed that DARPA sponsor, at U.S. companies, a minimum of four foundries or mini-factories to produce advance materials and components for military and commercial insertion, as laboratories to verify manufacturing principles, and for use in training and educating a competitive workforce. Each factory would have a companion university activity.

Develop the Principles and Systems for Implementing Concurrent Engineering

The sequential product realization methods have been shown to be costly, prone to errors, and totally ineffective in timely achievement of new product introduction. Simultaneous or concurrent engineering principles are evolving for assembly processes and for some metal fabrication processes. It is not currently a limiter in VLSI chip production. However, in most advanced materials and components manufacturing concurrent engineering is in its most rudimentary stages. Concurrent engineering is especially powerful when state-of-the-art CAD tools are coupled to process driven design rules. Great advances could be made if the process knowledge were coupled to the tools of concurrent engineering. It is proposed that a concurrent engineering program be funded to support each of the mini-factories and be defined by the specific needs of the selected products and processes.

Develop the Methods and Tools for Education and Training of the Workforce

It is unanimously agreed that in most U.S. firms the skill level of first level operators, and the knowledge and practice of manufacturing managers and

engineers is not on a par with world class manufacturers. It is also broadly accepted that well over 50% of the problem in achieving manufacturing excellence is in this non-technology arena. It is proposed that DARPA take a leadership role in the resolution of this critical problem. This research initiative should include programs (a) to facilitate the use of factories, including the research factories, as teaching factories for all levels of the workforce; (b) to develop software for teaching, computer-aided instruction, of the workforce (first level) in basic mathematics, statistics, simple principles of mechanics, physics and chemistry, etc.; and (c) to develop software for the improvement of foreign language skill especially Asian and East European.

Develop the New Standards and Metrics for World Class Manufacturing

There are standards and metrics for measuring products (although often primitive or inadequate); but there are very few non-financial standards and metrics for measuring manufacturing performance. The current business drivers ROI, ROE, ROA (return on investment, equity and assets) and quarterly profits are de-industrializing the U.S. New manufacturing metrics for allocation of resources, total factor productivity, complexity, time to breakeven, etc., would allow an enlightened cadre of managers to cause change and establish manufacturing excellence. The DARPA initiative for research in metrics will require interdisciplinary university research teams doing non-traditional research in U.S. and foreign manufacturing firms and in the DARPA research and teaching factories.

Manufacturing can evolve as a principle based discipline. DARPA can take a leadership role in creating a research structure that allows these new

rules and principles to be discovered. The opportunity is defined for DARPA to lead in the establishment of the new paradigm for advanced materials and components manufacturing.

II. INTRODUCTION

The manufacture of advanced materials and components offers one of the significant challenges to technologists and managers for the next several decades. The future DoD requirements for traditional and complex systems require components and subsystems made of advanced materials all of which must be accomplished in a budgetary environment of high quality and lost cost. The only resolution to these issues is a DoD supplier system capable of manufacturing excellence[15]. In fact, the future DoD requirements are precisely those of the commercial sector; and thus, a U.S. industrial base built upon companies that practice and drive world class manufacturing is the most important mission for DARPA at this time.[23]

Advanced materials and components have been universally identified as strategic capabilities for individual firms as well as the nation. The challenge for engineers and technologists is to implement the scientifically based product and process opportunities generated by the nation's R&D efforts. Key to this timely implementation is the creation and reduction to practice of principles for manufacturing. The complexity and diversity of manufacturing, which includes all of those processes involved in the creation of products through their production to their service in the field, have relegated the field to a collection of activities rather than a defined discipline. The purpose of the workshop was two fold: (1) considerable thought and analysis was required to identify the practices and rules of thumb which when verified through experimentation could become

principles, laws of manufacturing. The knowledge bases found in materials science, mathematics, fluid mechanics, system control, numerical simulation, etc., may form parts of the foundation for this future manufacturing science; (2) a small number of high impact opportunities were identified which could be defined as major DARPA initiatives and which provide demonstrations for manufacturing excellence.

Consider the manufacturing dilemma for an American firm. The growth of knowledge in materials science and engineering and the changing markets and customer requirements in material-using industries has changed fundamentally the demands placed upon firms in the advanced materials business. Contrast the situations facing advanced materials firms today with conditions in the era of bulk materials. In that environment, success depended upon large-scale, high-volume production of a widely used commodity material, where meeting shipment targets, reducing cost, and managing large capital assets was key to success. Meeting delivery requirements, reducing cost, and managing capital assets remain important in today's environment, but the challenges run deeper. Advanced materials firms must deal with a much broader range of customer demands, the levels of performance in the product demanded by customers are much higher and more specialized, the firms must respond to a changing set of demands more flexibly and faster than ever before, the the critical resources are less physical capital, and more the knowledge of customers, products, materials, and processes. This changing environment in components may be quite different in comparison to the 1950's. The challenge today is to achieve excellence in all of the activities involved in the design development, production, and distribution to customers. Moreover, excellent capabilities in a functional area must be integrated with other capabilities in the firm in order to

achieve superior overall performance. The critical functions in an advanced materials company include: (1) the acquisition and implementation of science and technology for advanced material products and processes; (2) a complete understanding of customer needs and, more broadly, emerging markets; (3) superior production capabilities, including product and process design and their implementation; and (4) effective organizations and systems for sales, service, and distribution. The changes in the paradigm to be emphasized here are the requirement for excellence in all facets of corporate enterprise and the assets now required for success. A focus on physical assets (the basis for advantage in the era of bulk materials) must yield to a new era in which knowledge, people, and flexible physical assets combine to yield strategic advantages when used for manufacturing excellence. <u>The definition of excellence and the principles and practices which underlie it remain the intellectual challenge of the future and the key to DoD and industrial competitiveness. (see Appendix A)</u>.

Table I most powerfully communicates the epochs of manufacturing practice and the changes in technology and practice[14]. Although this table looks at data for one firm, Beretta, the transformations in manufacturing have occurred throughout all industries. The "dynamic" world of manufacturing has been epitomized by the best Japanese firms and represents the principles which many American companies are trying to put into practice today. The "quality" paradigm with its requirement for understanding of the customer needs and for controlling manufacturing processes is implicit in the dynamic approach. It appears that firms must acquire this capability if they are to transition into the numerically controlled and the computer integrated manufacturing eras.

The Workshop examined those manufacturing fundamentals which would allow firms to catch-up (known principles not needing research) and fundamentals which require a research agenda to discover and implement

knowledge-based manufacturing principles in to advanced materials and components design and production. This is described schematically in Figure 1.

TABLE I. The historical changes in manufacturing practice at the Beretta arms manufacturing company (after R. Jaikumar).

MANUFACTURING SYSTEM	English System	American System	Taylor Scientific Mgmt.	Dynamic World	Numerical Control	Computer Integrated Manufacturing
BEGINNING OF PRACTICE	1800	1850	1900	1950	1960	1980
ENGINEERING ETHOS	Mechanical	Manufacturing	Industrial	Quality	Systems	Knowledge
PROCESS FOCUS	Accuracy	Repeatability	Reproducibility	Stability	Adaptability	Versatility
FOCUS OF CONTROL	Product Functionality	Product Conformance	Process Conformance	Process Capability	Product/ Process Integration	Process Intelligence
INSTRUMENT OF CONTROL	Micrometer	Go/No-Go Gauges	Stop Watch	Control Chart	Electronic Gauges	Professional Workstation
ORGANIZATIONAL CHANGE	Break-up of Guilds	Staff/Line Separation	Functional Specialization	Problem Solving Teams	Cellular Control	Product P3 Process Program
WORK ETHOS	"Perfection"	"Satisfy"	"Reproduce"	"Monitor"	"Control"	"Develop"
SKILLS REQUIRED	Mechanical Craft	Repetitive	Repetitive	Diagnostic	Experimental	Learning Generalizing Abstracting
NUMBER OF MACHINES	3	50	150	150	50	30
MINIMUM EFFICIENT SCALE (NO. OF PEOPLE)	40	150	300	300	100	30
STAFF/LINE RATIO	0:40	20:130	60:240	100:200	50:50	20:10
PRODUCTIVITY INCREASE OVER PREVIOUS EPOCH	4:1	3:1	3:1	3:2	3:1	3:1
REWORK AS FRACTION OF TOTAL WORK	0.8	0.5	0.25	0.08	0.02	0.005
NUMBER OF PRODUCTS	Infinite	3	10	15	100	Infinite

World class manufacturing (WCM) or manufacturing excellence is a newly discovered term in America's competitiveness and productivity jargon. It represents the re-discovery of how important the "marking of things" is to our economy and our total infrastructure. The careful examination of eight major industrial segments to determine root causes of non-productive practice and loss of competitiveness showed remarkable consistency between firms which are the very best and those which are suffering[2]. This study and others[7,8,24] suggest that even with the current U.S. disadvantages with its macro-economic and political environment, these are strategies for manufacturing excellence. Many of these are consistent with initiatives DARPA might undertake in advanced materials and components manufacturing.

Whether in Japan, Europe or the U.S., world class manufacturers can be recognized by[8]:

1. Being the best competitor in their industrial segment and being superior in most functions which comprise the manufacturing enterprise. (WCM cannot be good in just one function; e.g., innovative product design.)
2. Being more profitable and growing more rapidly than competitors -- superior products and long term measurements (profit) to prove it.
3. Hiring and retaining the best people and investments in programs to improve their skills; a work-force that others are always trying to "steal".
4. Development of an engineering staff which are so expert in product and process, in systems and software, etc., that vendors and suppliers (production equipment, computer services, etc.) continually seek advice about improvements and modifications to their own offerings

and request that the WCM be the test site for new equipment, systems and pilot models.

5. Being able to respond quickly and decisively to changing market conditions; market not marketing driven; nimble enough to play niche as well as large markets.
6. Intertwining the manufacturing functions (engineering design, R&D, manufacturing, marketing, etc.) to create a seamless organizational atmosphere and with tools, methods and measures which support the total enterprise performance.
7. A total commitment in word and deed to continuous improvement of people, facilities, product, processes, organization, strategies, etc.

These standards define opportunities for firms to improve (Figure 1) and become excellent by today's criteria. The concepts described in Table I and shown schematically in Figures 1 and 2 suggest additional approaches will be required to be in the league of world class in the mid-to-late 1990's. These are the topics for research and development.

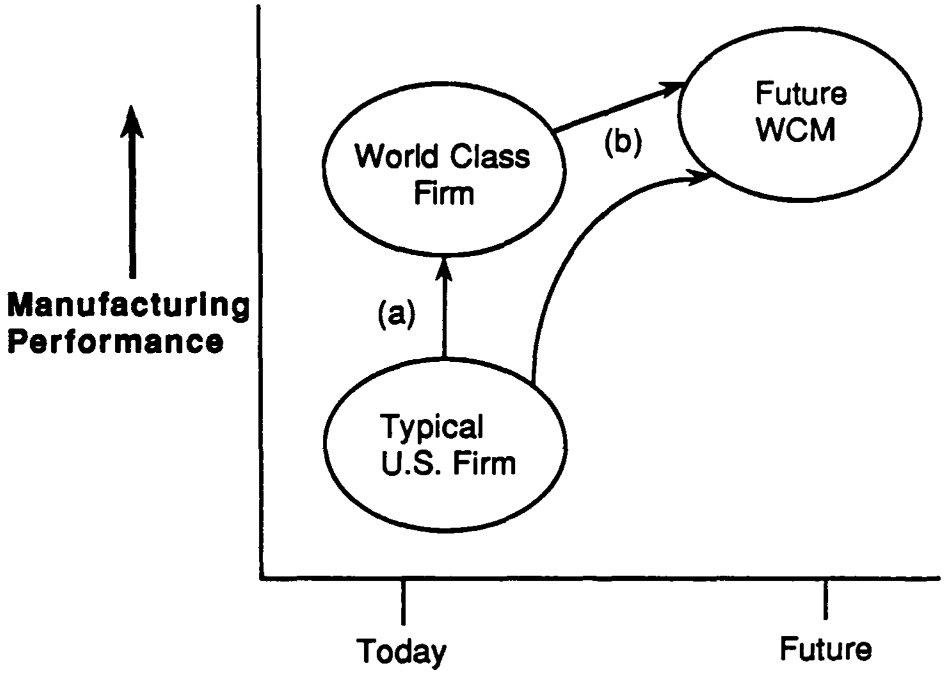

Figure 1. Schematic representation paths to improve manufacturing performance through the application of (a) known rules and (b) newly discovered principles.

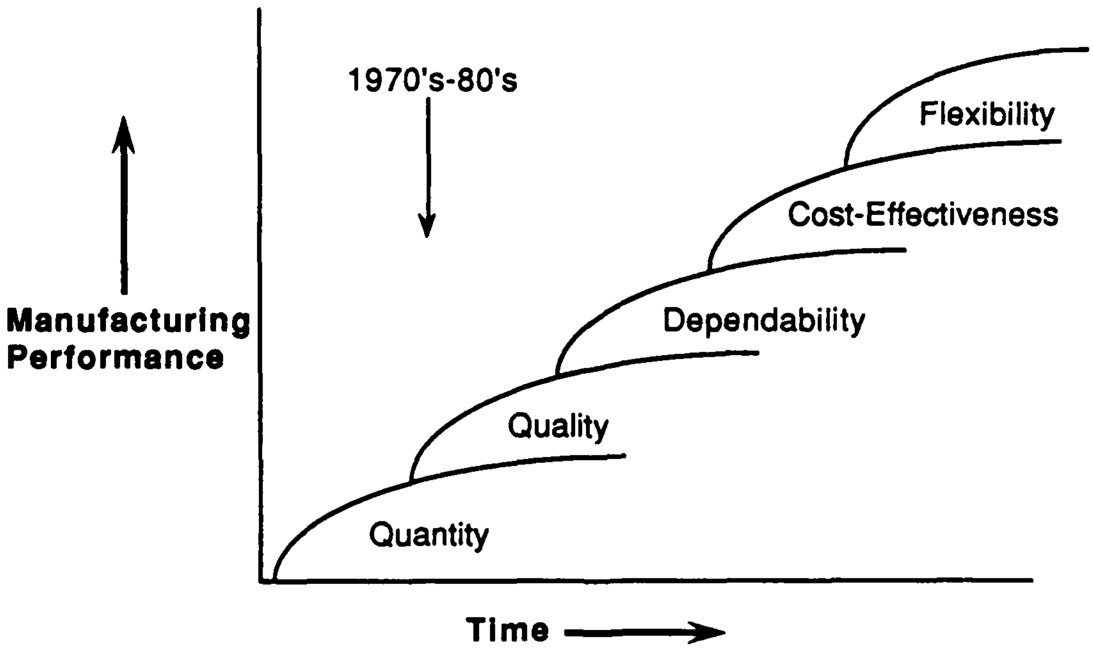

Figure 2. Schematic representation of the changing metrics of manufacturing performance.

III. BACKGROUND INFORMATION FOR THE WORKSHOP

The background information and intellectual input for the Workshop came from pre-meeting readings (see bibliography), formal presentations from industry experts, and responses to a questionnaire. The experts were chosen because of their extensive experience base in all materials classes and in materials and components for numerous functions (optical, structural, electronic, etc.) and in various engineering systems. The specific needs for each technology base manufacturing system may be different but the overall issues and problems appear to be very similar. This consensus also extended to requests for research to establish a manufacturing science through formal research procedures to establish fundamental principles, methods and practices.

The formal presentations were given by:

Dr. Harry Cook, Director of Technology, Chrysler Motors Corp.

Dr. Philip H. Francis, V.P. Technology, Square D Company
(also editor of the journal - Manufacturing Review)

Dr. Scott Elliott, Manufacturing Manager, Hewlett Packard Microwave
Technology Division

Dr. James D. Dowd, formerly Director of Manufacturing Research,
Alcoa

Mr. Joseph Yanus, V.P. Manufacturing, Alcoa AIX Division for
Electronic
Packaging (formerly manufacturing manager, IBM East Fishkill)

Dr. Hans Verleurs, Manufacturing Operations Manager, AT&T
Lightwave Products Division

Mr. Joseph B. Moore, Director of Materials Engineering, Pratt and
Whitney Government Engine Business

Prof. James Mar, Aeronautics and Astronautics, MIT (senior advisor on structures and composites to major airframe manufacturers)

Dr. Michael Jaffe, Fellow, Hoechst Celanese Research Division

Prof. K.K. Wang, Director of the Industry Consortium Injection Molding Program, Cornell University

Prof. Willis Adcock, Materials and Manufacturing, Univ. of Texas (formerly senior technology manager, Texas Instruments)

Dr. Robert C. Pfahl, Jr., Director of Manufacturing Research, Motorola General Systems Group

Prof. Hayden Wadley, Materials Science and Engineering, Univ. of Virginia

Dr. Philip Parrish, V.P. Concurrent Engineering Technology, BDM Division of Ford Aerospace

The experts and MRC/DARPA participants were asked to respond to the questionnaire reproduced below:

QUESTIONNAIRE

Six weeks in advance of the Workshop, the expert guests and a few MRC members, were asked to complete the following document.

DARPA MATERIALS RESEARCH COUNCIL

FUNDAMENTALS OF MANUFACTURING: ADVANCED MATERIALS AND COMPONENTS

JULY 11/12 Workshop, La Jolla, California

Definition of "Manufacturing" for the purposes of the Workshop:

Manufacturing includes all of the hardware, software and humanware knowledge, processes and systems for making advanced materials and components. Thus manufacturing may range from the product/process development (applications of science and engineering principles), to the production processes and facilities operations and finally to the sales and field service.

____

Name

BASED ON MY EXPERIENCE:

A. World-class manufacturing of ____________________________is driven by the following key technologies:

Business success as determined by non-financial metrics for world-class manufacturing are:

B. The most significant requirement in the future to successfully compete in this market is:

C. My list of "Manufacturing Rules" includes:

D. The Manufacturing Rules which could drive companies in my industry to practice manufacturing excellence if these rules were better documented are:

E. The characteristics of the person I would hire to lead the development and implementation of my next product/process are:

F. The future DARPA Research Agenda should include:

1. Research thrusts verify "manufacturing rules" such as:

2. Research thrusts to invent and innovate the next generation "manufacturing rules" such as:

3. Special targets (large projects?) such as:

IV. KNOWN RULES FOR MANUFACTURING

The examination of the literature and the accessing other efforts[1] directed to identify fundamental principles for manufacturing in combination with contributions of the Workshop participants led to the generation of a list of rules which are practiced by WCM (World Class Manufacturing) firms. In almost all cases, the validity and boundary conditions have not been carefully tested. Many are more primitive in form, i.e., admonitions, while some are more formal and a few take on the form of equations.

The proper implementation and practice of these rules appear to be minimum level indicators of manufacturing excellence for a distinguished set of firms. These known but still not widely accepted rules are:

1. Technology applications to achieve WCM are enhanced after or in conjunction with the implementation principles of total quality management.
2. The quality/cost ratio cannot be maximized by relying on final product inspecting; i.e., sorting.
3. Manufacturing excellence is proportional to the quality (skill-base and continuous improvement of) and effectiveness (total quality management) of the work force.

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[1] e.g., Study Groups of the NRC and NAE.

4. Maximum process yields are achieved through self regulating processes.
5. Provide incentives for process improvement at all levels; empower the first-line operators. Discover and control critical processes.
6. The slope and level of the manufacturing learning curve are a function of the quantitative process understanding.
7. It is imperative to gain a thorough understanding of the customer and the customer needs.
8. Upstream variability is more difficult to control and compensate for with downstream processes; e.g., raw material composition, purity and reproducibility must be maintained to simplify downstream manufacturing process.
9. If a process does not reduce inventory, increase throughput, increase quality or add to the product performance, then do not do it.
10. Decreasing variability reduces cost. Corollary: Reducing variability improves performance.
11. Cost is an increasing function of complexity.
12. Little's law, $I = l(W + 1/m)$, which relates the mean in-process inventory (I) to the mean waiting time (W), the mean time to process (1/m), and the mean movement rate (l).
13. At equilibrium: output $\leq$ input; output rate $\leq$ input rate.
14. Optimization of the values of the sub-system $\leq$ optimization value of the total system.
15. An optimized process cannot be improved later by adding constraints.

16. In synchronous processes:
    a. for low to medium work-in-process (WIP) the production capacity (PC) = WIP inventory (WI).
    b. for higher WIP: d(PC)/d (WI) is less than one and tends toward zero.

V. MANUFACTURING RULES WHICH REQUIRE FURTHER STUDY, CLASSIFICATION, AND CODIFICATION

There are a number of manufacturing tenets and rules that Workshop participants believed to be true but for which the data have not been accumulated. Many of these are practiced by WCM firms but the full understanding and definitions of applicability have not been documented. For this set it is recommended that case studies and other methods of comparative examination be made using the rigorous study methodologies of an NRC type study group. These rules which need clarification, classification and codification include:

1. The firm's manufacturing strategy is a critical component of its corporate business strategy.
2. Maximizing quality will reduce costs.
3. The ultimate economy of scale is a lot size of one. Corollary: Manufacturing competitiveness is independent of volume.
4. Responsiveness and productivity (not defined in the narrow traditional sense of labor hours per unit produced) is directly related to flexibility.
5. Minimization of waste (in all forms) increases quality.
6. Maximize the enterprise total factor productivity.

7. The manufacturing capability and quality index is highest for systems which are able to operate with minimization of defects, lot-size, set-ups, handling, lead time, breakdowns and surges.
8. Optimize the value-added in all manufacturing processes and functions.
9. The product design and the product design process have a very large direct effect on the production process; specifically issues of time, cost and quality.
10. Minimize toxic wastes, waste streams, and occupational hazards; use life-cycle costs as the metric.
11. Manufacturing excellence (total factor productivity, quality, flexibility) requires division-level (plant-level) capabilities in the development and improvement of equipment, machines, software, systems, etc.
12. Quality (products, processes, systems, organization...) must be quantified and measured in order to drive WCM.
13. Critical manufacturing tools and methods include parameter searches, multi-variable response surfaces, etc., but the most powerful tools are based on fundamentals (physical laws, statistical methods, empirical laws, verified non-financial metrics,...)
14. While long-term profitability, market share and growth are the goals of a manufacturing firm, quality, cost, time and flexibility are the principle metrics of WCM linked (cell) processes, etc.); and

15. There are system specific procedures and principles which describe how information and knowledge about product and process should be used -- examples are:

   a. the data and information hierarchy and strategy for CIM (Control In Manufacturing) (process control, cell-level, etc.) implementation;

   b. the order of activities for integrating a manufacturing line (product simplification, process simplification, statistically controlled processes, computer controlled processes, computer linked (cell) processes, etc.); and

   c. the difficulty of managing complexity and implementing (introducing) technology: insertion of new materials preferably with known equipment or new product with functioning line or a new process equipment to produce a current product.

VI. WORKING GROUP REPORTS

The efforts to identify fundamental principles for manufacturing also led to specific research needs requiring the development of a set of rules for to future WCM. These rules require rigorous research and a unique multi-disciplinary environment unlike most government sponsored programs. The issues are, however, very much in the style of past DARPA initiatives. The research needs were grouped into four themes which would lead to advanced materials and components manufacturing principles.

Workshop participants formed four Working Groups to use the data and information established in the Workshop and which had evolved into a consensus statement, and to develop a structure for resolution of the research

questions. The output of the Working Groups reflects these four themes:

A. Process Knowledge & Control

B. Concurrent Engineering

C. Management, Education and Training

D. Manufacturing Metrics

A. WORKING GROUP ON PROCESS KNOWLEDGE & CONTROL

Participants:

J. D. Dowd, A. G. Evans, G. Farnum, R. Mehrabian, J. Moore, R. C. Pfahl, H. Wadley, K. K. Wang, G. Whitesides, J. Yanus

PROBLEM STATEMENT:

Process knowledge and control, embedded within a robust information system, are essential elements of a WCM capability. In general, Japanese companies spend twice as much on process development as on product development while U.S. firms spend twice as much on product rather than on process development.

1. Process control is a necessary but not sufficient element of WCM. The real differentiator, beyond catching up to the Japanese, is the close coupling of process knowledge with control. The application of process understanding, e.g. predictive models, will permit the flexibility in process development/improvement not available though standard control schemes presently practiced to reduce variability (Figures 3 and 4).

A robust information system is an enabler to enhanced process understanding and control. At present, most process variables are tracked and related to specific characteristics of the product. In a robust information system this data is continuously captured, and cross-correlated on a local unit process scale as well as higher levels of the processing hierarchy. A primary aim is to learn about the process, understand it more fully, by viewing the plant environment as a dynamic development organization.

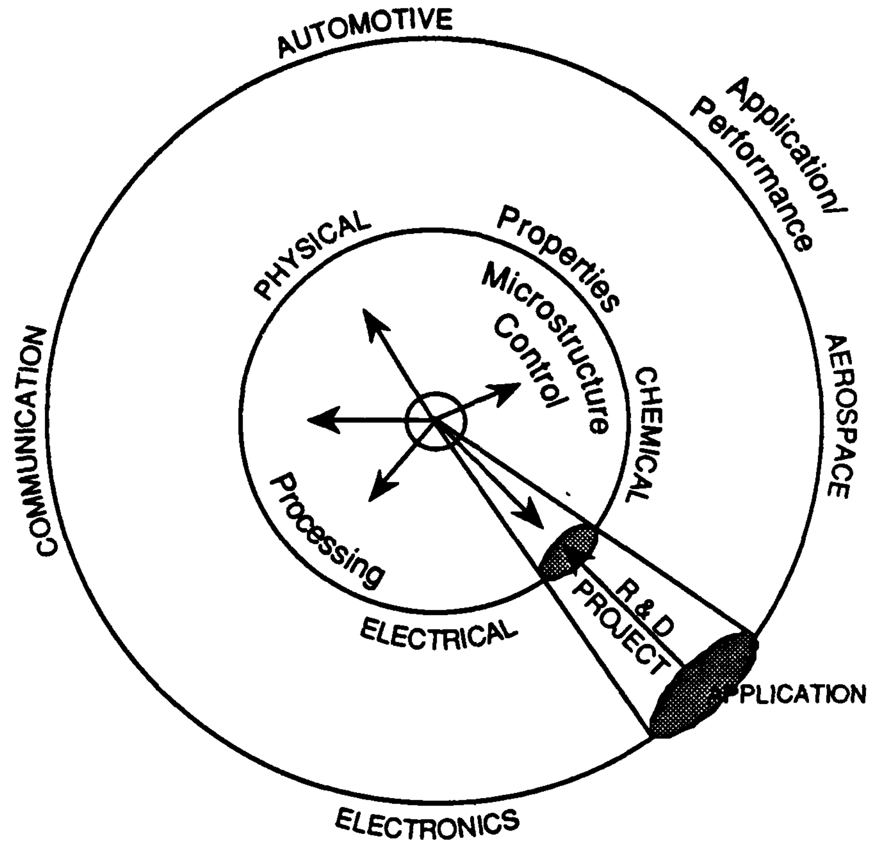


Figure 3. The past approach to product realization started with the application, then product design and finally processes for manufacture. The new approach establishes rich process technologies applicable to a wide range of products. Process knowledge allows for process driver product design.

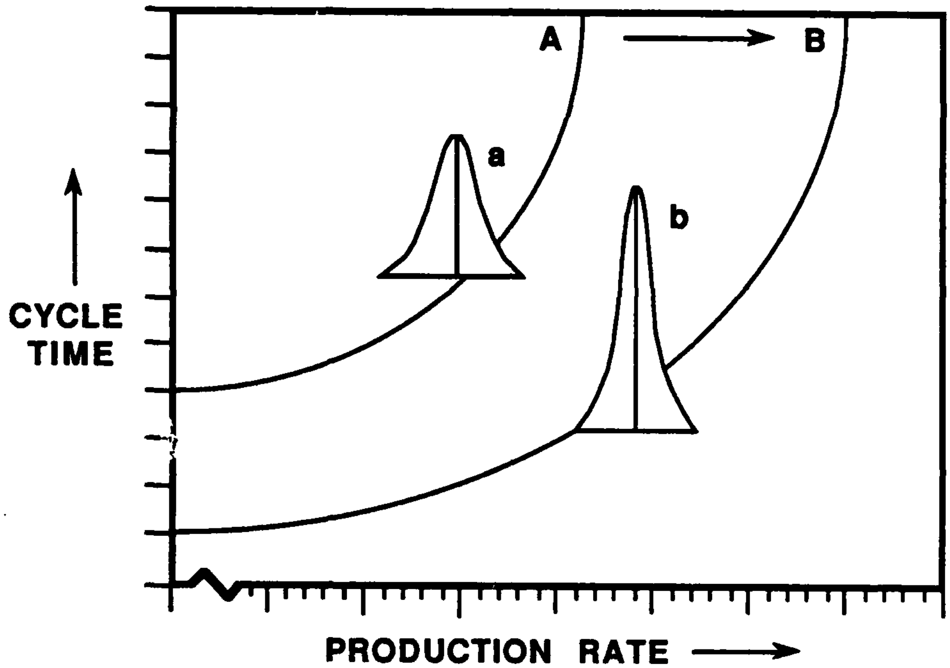


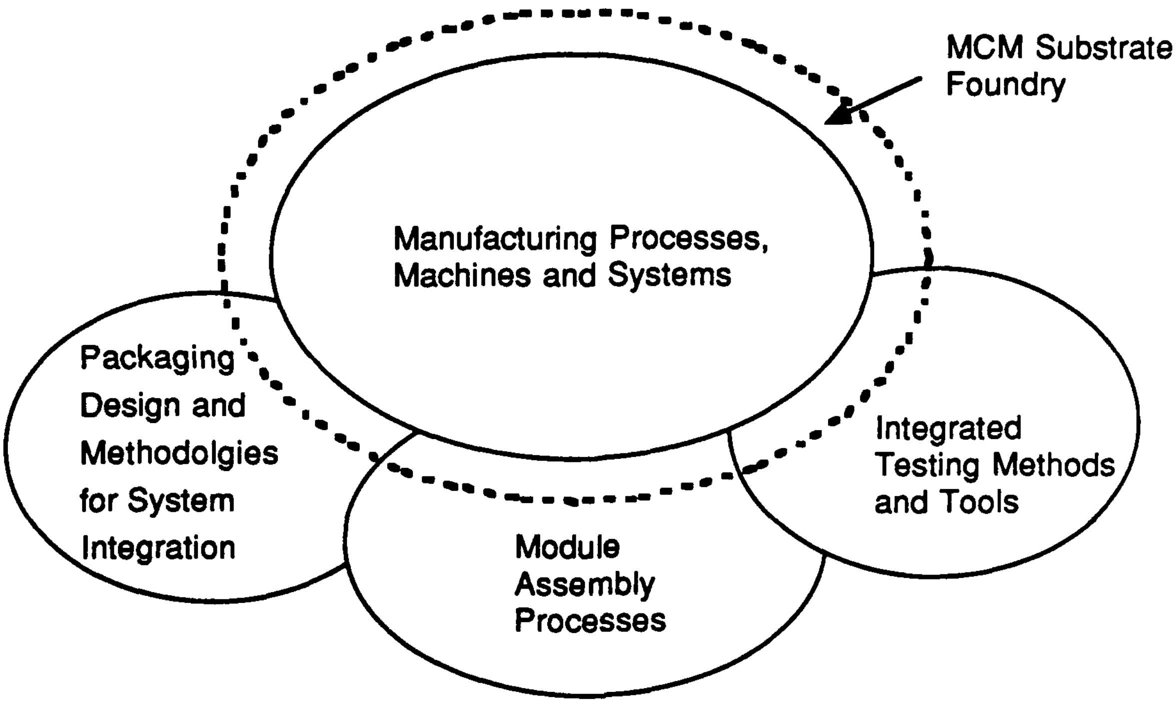
Figure 4. Process control and process knowledge (narrower distribution or process parameters in b than in a) allow for improved product introduction cycle times and a wider range of low cycle times even for large production rate requirements (after W. Adcock).

2. Possible candidates for development of a WCM facility by DARPA as a model for U.S. manufacturers were discussed. Three generic manufacturing enterprises based on technology content, importance to U.S. competitiveness and DoD were identified: (a) Electronic Packaging, (b) CVD/CVI Composites and Coating, and (c) Composite Joining. The first two were the subject of extensive discussion and all three were proposed for further consideration and discussion by the MRC and DARPA personnel.

Electronic Packaging: Multi-chip Module (MCM)

A DARPA manufacturing program is proposed to innovate the next generation of process/product/material technology and associated process knowledge and control for packaging of electronic components *which meets the product needs of high performance*, compact size, and low cost. The program elements would include:

1. Design Methods and Tools (thermal, mechanical, and electrical).
2. Intelligent Manufacturing Control (sensors, process simulation, models, machines) for the substrate (ceramic-metal) and signal layers (polymer-metal).
3. Information Integration (process driven design rules CAD/CAM, test, production,etc.)



CVD/CVI Composites/Coatings

CVD/CVI are critical technologies for the production of coatings, fibers, and high temperature structural composites. Application of process knowledge and control schemes in the CVD processes are used in the micro-electronics industry. Transfer of these methodologies to the structural materials application of CVD/CVI should permit rapid development of a WCM via a demonstration facility. The program elements would include:

1. IPM Process Knowledge and Control System:
   a. Development of process understanding based on flow models, high temperature chemical reactions, kinetics, and thermodynamics.

b. Development of methods to measure in-process-product attributes such as open and closed porosity, adherence, modulus, etc.

c. Development of process sensors (density, gas composition, temperature, pressure, etc.)

2. Production knowledge - use the production system developed in (1) to fabricate parts and test the manufacturing system aspects. This will require hundreds of production runs.

Composite Joining

Although the large scale production of resin matrix composites is yet to be realized, there are strong indications that these manufacturing systems are possible as design tools and process knowledge come together. A key missing technology is that related to manufacturing processes for joining composites which do not involve holes and fasteners similar to metal joining. Polymer matrix composites bonding offers another unique DARPA opportunity and again it would focus on intelligent manufacturing processing and control: design/failure criteria; in-process monitoring; physical/chemical modelling; methods for dimensional control; etc.

BACKGROUND: Process Knowledge and Control

All participants in the Workshop contributed to a list of key rules of manufacturing which needed research to establish their validity. These are process knowledge rules which could be verified for specific products and processes in a unique DARPA sponsored program. The rules which need to be studied include:

1. Process knowledge (the real differentiator) and process control (the minimum price of entry) are essential elements of WCM and empower the key metrics of quality, cost, time and flexibility.
2. WCM requires division-level or plant-level capabilities in the development of next generation equipment, machines, software, systems, etc.
3. Production data and the tools and methods to transform data to information and knowledge, provide invaluable resources for product/process improvements and innovations.
4. Process knowledge including all aspects of materials transformations (physical-chemical processes, equipment and system operations, etc.) provides the foundation for process driven design, rapid prototyping, shortened time to break-even, concurrent engineering, etc., methods and tools focussed on the new metrics of WCM.
5. Advanced materials and components manufacturing processes and systems require flexibility - composition tolerant and shape independent.
6. Non-invasive sensors and process monitors (temperature, pressure, composition, position, flatness, density, etc.) will enable future WCM of advanced materials.

B. WORKING GROUP ON CONCURRENT ENGINEERING

Participants: P. Parrish, K. Adams, H. Cook, A. Patera, T. Kailath, J. Yanus, R. Sheridan, J. Rice, M. Jaffe

PROBLEM STATEMENT:

The sequential product realization methodology commonly practiced by industry (R&D -> design -> manufacturing -> maintenance and logistics) leads to designs that do not adequately consider manufacturing, maintenance and logistical issues in the preliminary design phase. This results in costly redesigns, frequent engineering change orders, loss of design intent, increased cost and time to product introduction, and compromises in product quality. (Figures 5 and 6) This has a strongly negative impact on timely ability to achieve market share, and adversely affects U.S. competitiveness in global markets. Loss of competitive edge, in turn, diminishes the U.S. defense industrial base.

The concept of concurrent engineering (CE) seeks to enable simultaneous consideration of all major factors in product realization and application, enabling rapid prototyping of designs and products through teaming between designers, manufacturers, and logistics, maintenance and other support functions. This has been demonstrated on numerous occasions in small "tiger-team" or skunk works projects. DARPA's Initiative in Concurrent Engineering (DICE) has completely specified and is developing a CE information management system to enable distributed teams to conduct rapid product development utilizing a systematic approach where product intent and requirements interplay with process, organization, time, cost and other constraints and resources. Concurrent, cooperative efforts between

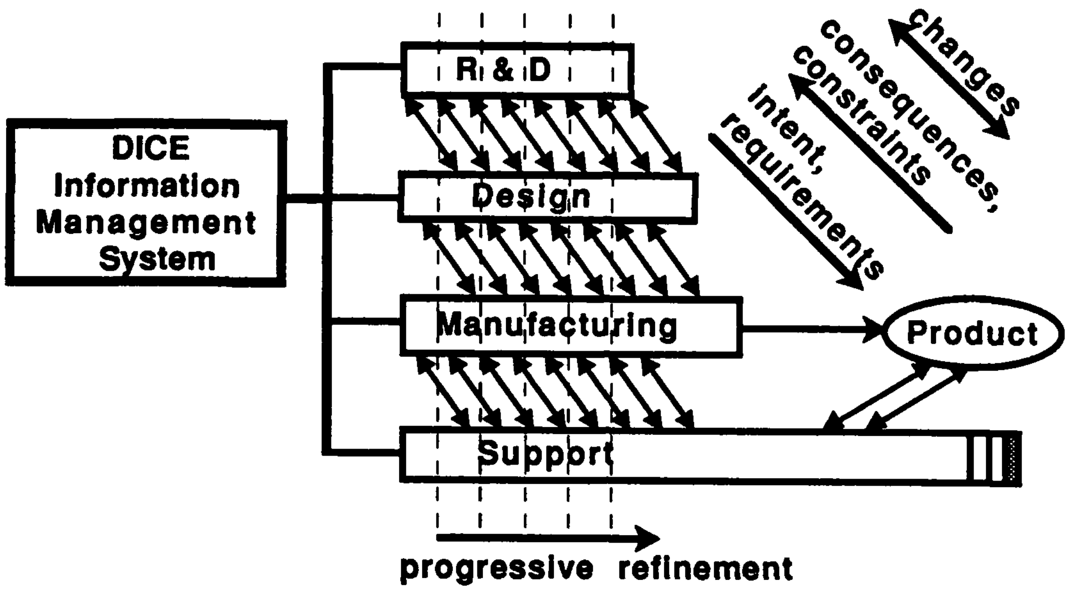


Figure 5. Schematic representation of DARPA's Initiative in Concurrent Engineering (DICE) stressing parallel as opposed to sequential processes.

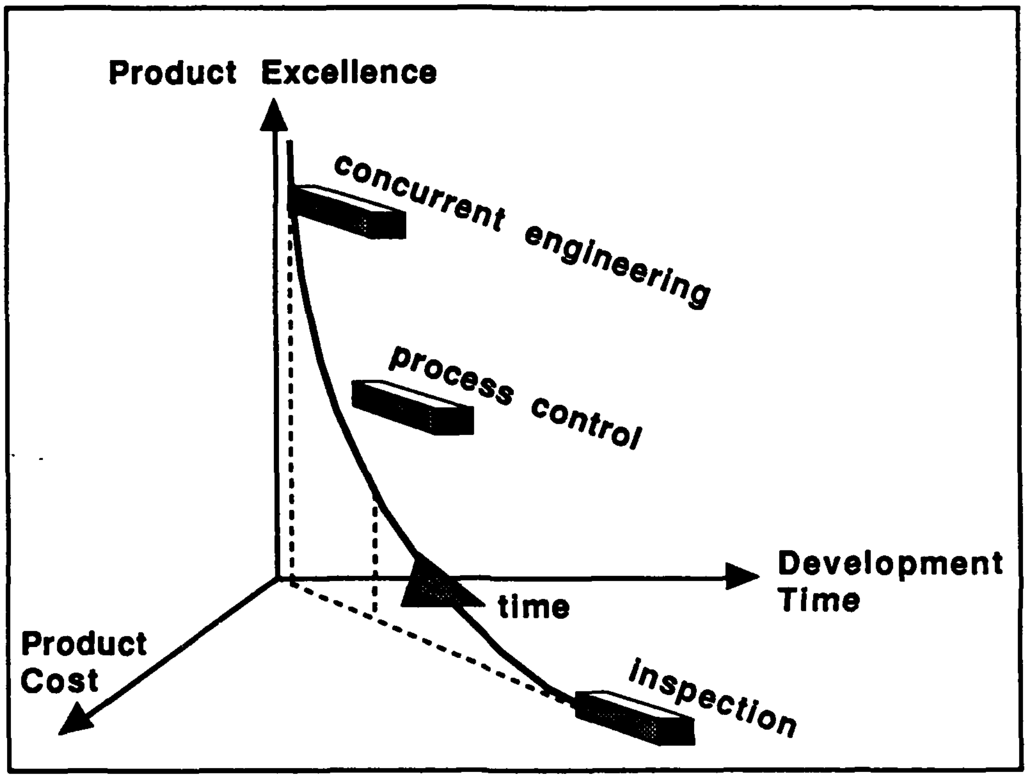


Figure 6. Representation of the improvements in product excellence, cost and development time through proper implementation of concurrent engineering.

engineering, marketing, manufacturing and field entities utilize the DICE system for conceptual design, evaluation and progressive refinement considering all viewpoints, and managing resources, risks and product optimization without loss of product intent. The enabling technologies for CE include object-oriented system design, high power computer workstations, information modeling and standards. Critical bottlenecks are feature-based design language and data bases, solid modeling capabilities with high-rate graphical generation for local feature editing in conjunction with automated mesh generation/regeneration for finite element analysis (e.g., local stress and thermal analysis) to enable automated representation of relevant materials and process selection alternatives for cost-effective design and production.

RESEARCH

A DARPA program is recommended to develop networks of prototype concurrent engineering workstations, based upon the DICE architecture, and focused on applications and demonstrations in three major areas:

1. high density electronic packaging
2. composite material structures and tooling design for manufacturing
3. assembly of advanced electro-mechanical systems (e.g., avionics packages)

Each of these demonstrations would include development of central data base architectures for each domain, object-oriented product and component descriptions based upon features, automatic numerical control generation, and the ability to deal with hierarchical issues of representation and interaction at the systems, subsystems and component levels.

BACKGROUND: Manufacturing Rules for Concurrent Engineering

The above research program came from the identification by all Workshop participants of a set of research questions. These were viewed to allow significant advances in our productivity and competitiveness. Concurrent engineering research is needed to establish the principles and practices for advanced materials and components manufacturing. The rules which need to be studied and codified and which would have major impact for future WCM are:

1. What are the software, hardware, organizational, and systems aspects and the underlying principles for concurrent engineering? Clear definitions and tools - what; specific mechanisms for implementation - how; and the impact-metrics are required to move this field from a curiosity to key practice of competitive U.S. Firms.
2. What are the product/process specific "design for ---" principles, methods and measures? Can we move from higher level design principles (e.g., design for assembly) to detailed and physics based design principles (finite element analyses)? Can these design principles really be manufacturing process driven and interactive?
3. What are the model product/process experiments which will allow DARPA to demonstrate the full potential of computer technology to the total manufacturing enterprise? For example, research is needed to establish a common data base (within the manufacturing firm and its vendors and customers) and seamless computer software interfaces between corporate functions (engineering - manufacturing - MIS) or amongst design and analysis methods (electrical, thermal or mechanical design).

4. Since time and flexibility will be the key new differentiators for WCM, we need models, demonstrations and metrics from research on specific advanced materials and components which creates this new knowledge base. Examples of specific projects include a rapid prototyping facility for structural ceramics components or of tools and molds (for plastics or metals casting); a concurrent engineering system for resin matrix composites; or detailed analyses of a current set of products/processes to establish metrics for time to break-even.

C. WORKING GROUP ON MANAGEMENT, EDUCATION AND TRAINING

Participants:

S. Elliott, H. Verleur, D. Srolovitz, J. Economy and J. C. Williams

PROBLEM STATEMENT:

A fundamental principle for WCM is that technology and technology solutions represent much less than 50% of the issues, problems and solutions. The corporate strategy, management principles, organization at the firm, and quality of the total work force have minimum requirements before product/ process technologies can be effective. It is imperative that the scope of the problem of manufacturing excellence be addressed in any DARPA initiative and that innovation methods be discovered to achieve these broad goals.

Given the extensive input from the literature and from the Workshop participants, this working group considered the need to improve the manufacturing work force and ways to accomplish this. A constraint which was placed on the range or scope of the discussion was that it should largely focus on areas where a DARPA initiative could make a significant contribution.

The new elements of research which would facilitate understanding of manufacturing fundamentals include:

1. A few model experiments which use or create the factory environment and which allows for studies of people and organizations within advanced materials manufacturing systems (software and hardware). Firstly, an understanding of complexity and secondly methods for dealing appropriately with complexity will need to be studied in order to determine improved

organizational methods and the principles and practices and for educating the total work-force (operators, managers, engineers, etc.).

2. In view of DARPA's long standing leadership in computing activities, an effort in computer based foreign language skill improvement and machine translation of foreign language documents (especially the Asian languages) would be very useful. With the increasing global focus of business, facility with foreign language has growing importance. In addition, an effort is needed to effectively translate the data from world wide sources into useful information.

3. Another area where DARPA's established leadership in computing could pay off is in the area of computer aided instruction (CAI). The effective tools for teaching the work force would fulfill an absolutely critical need and meet national requirements for an upgraded work force.

RESEARCH

The Working Group focussed on the formulation of one concept which would allow DARPA to take a leadership role in manufacturing education. All Workshop participants were emphatic that a major issue in our competitive position in manufacturing is centered around the training and quality of the manufacturing work force, including managers, engineers and hourly workers. A concept which would permit the attraction and preparation of engineers for careers in manufacturing is that of a Teaching Factory. DARPA should establish several teaching factories which reinforce the key materials and manufacturing technologies and organizational modes which will drive improvements in methods and practices through careful experimentations. The elements of this concept are outlined below.

Concept

The Teaching Factory (TF) bears some similarity to a teaching hospital in that its focus is on the preparation of human resources for careers in the manufacturing work place. In order to be credible the TF must produce at least limited quantities manufactured components, just as a teaching hospital is a real hospital.

Issues

The following issues related to the TF Concept were discussed and some suggested solutions were identified.

Students - Level: The students should have a minimum of a 4 year engineering or science degree.

Source: The students could be hired by companies and sent to the TF as a manufacturing "finishing school" or they could be existing company employees selected for attendance.

Activity - The TF activity would have to be focused on an area of manufacturing or particular technology area. In the electronics area the TF might see affiliation with Sematech.

Facility - The facility would be located at or near both a real manufacturing activity and a university. The physical facility would be provided by a company or through the state or local economic development effort or by some other (non-federal) means.

Funding - The TF would require funding to initiate it and to allow it to attract other funds. The notion is that DARPA funding for 3-5 years would be required during which time the amount of state economic

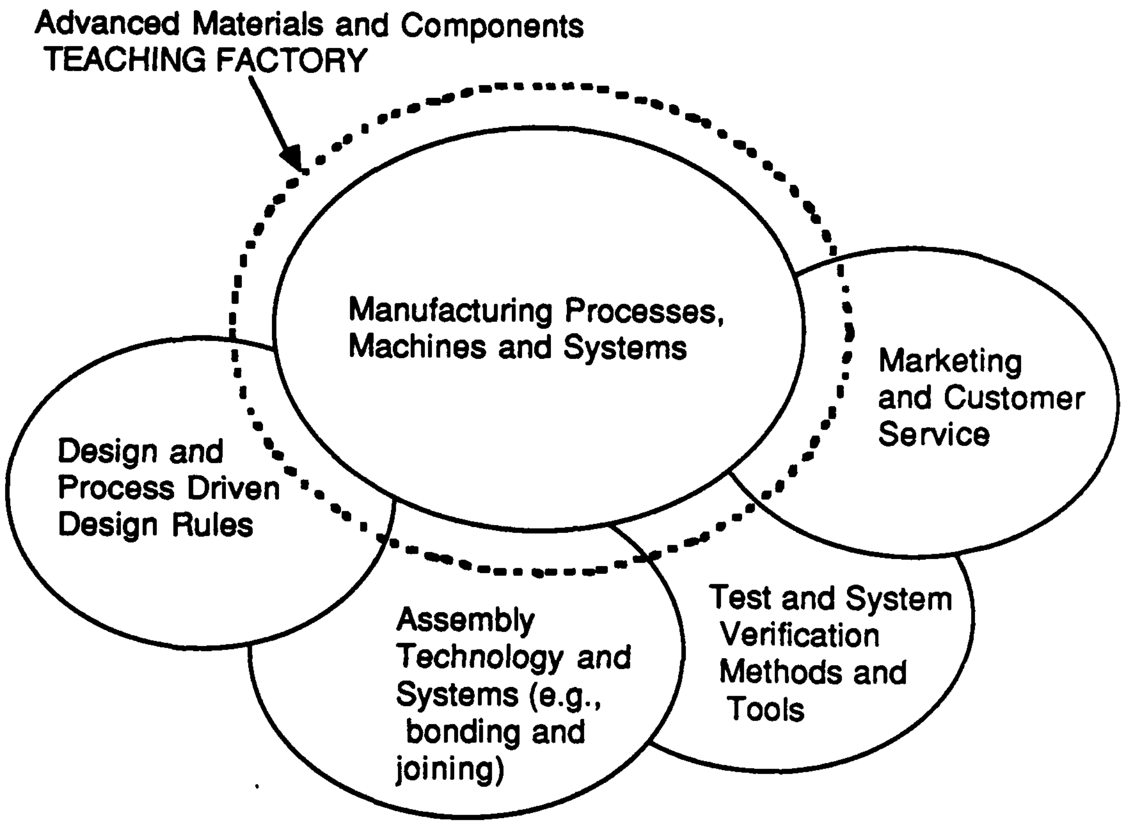
development and private sector funds would increase so that the TF becomes self-sufficient without ongoing DARPA funding.

Tax/Legal - The TF would be incorporated as a non-profit activity possibly a 501C3 corporation. Other issues related to intellectual properties will require attention and thought.

Output - The TF will produce qualified manufacturing engineers and a limited quantity of real product. The use of simulation methods to supplement the actual production should be examined as this appears to be attractive.

Other Issues Related to Education

There was also a suggestion that DARPA could take a pro-active role within DoD to establish a funding mechanism for defense contractor employees to be educated in manufacturing. This could be done by allowing part of the cost of educating manufacturing employee to be recovered as part of the overhead pool.The IR&D cost recovery system could be used as a possible model for implementing this.


Advanced Materials and Components
TEACHING FACTORY
Manufacturing Processes,
Machines and Systems
Marketing
and Customer
Service
Design and
Process Driven
Design Rules
Assembly
Technology and
Systems (e.g.,
bonding and
joining)
Test and System
Verification
Methods and
Tools

D. WORKING GROUP ON MANUFACTURING METRICS

Participants:

H. K. Bowen, P. Francis, D. Ferry, and J. Margrave

PROBLEM STATEMENT:

Today's manufacturing practice is perceived to be an art, a collection of functions and activities. WCM will require a manufacturing science that will allow; e.g., date driven, knowledge-base decisions for resource allocations. Research is needed to define and to quantify the metrics which will allow:

1. Quantification of continuous improvement of methodologies and procedures applicable to software, hardware, humanware, organization, strategic plans, etc.

   Examples of metrics are:

   a. Software -- user-friendly, ease of communicating to other software, improvements to visualization of information and issues, level of defects, inherent capabilities to cause individual and group learning, adaptability, ease of support, modularization, etc.

   b. Hardware -- operator-friendly, repairable/maintainable/ adaptable, amenable to closed-loop control, inherent stability, ease of built in sensors, monitors and testing, modularity/ structured design, etc.

2. The quantitative measure of and principles for managing complexity of products, processes, systems and organizations are key to WCM. Three typical domains of complexity are: (i) product development; (ii) manufacturing process systems; and (iii) internal (firm) communications.

Example metrics which may be applicable are:

a. information content; openness to flow of information;

b. natural tolerance to defects and errors;

c. robustness for ambiguity;

d. fidelity, bandwidth or error rate of processes;

e. timeliness;

f. degree of commonality of data bases (relational);

g. degree of commonality, where appropriate, of standards, procedures, processes and tools;

h. accessibility (lowest level accountability).

3. "Time" is an increasingly important measure of WCM and this recognition requires new principles, methods and measures for; e.g., (i) concurrent engineering, (ii) rapid prototyping, (iii) break-even time, and (iv) response to customers needs.

Typical issues which affect the needed metrics are:

a. full utilization of facilities (e.g., 24 hrs.) and assets;

b. effective use of the enterprise data base;

c. symbiotic user-vendor relationships;

d. product/process modeling and simulation;

e. enterprise simulation and business forecasting; and

f. transition point from pre-production test and verification of a manufacturing line to routine production.

Some of these are shown in Figure 7 for the particular case of manufacturing development of a new polymer.

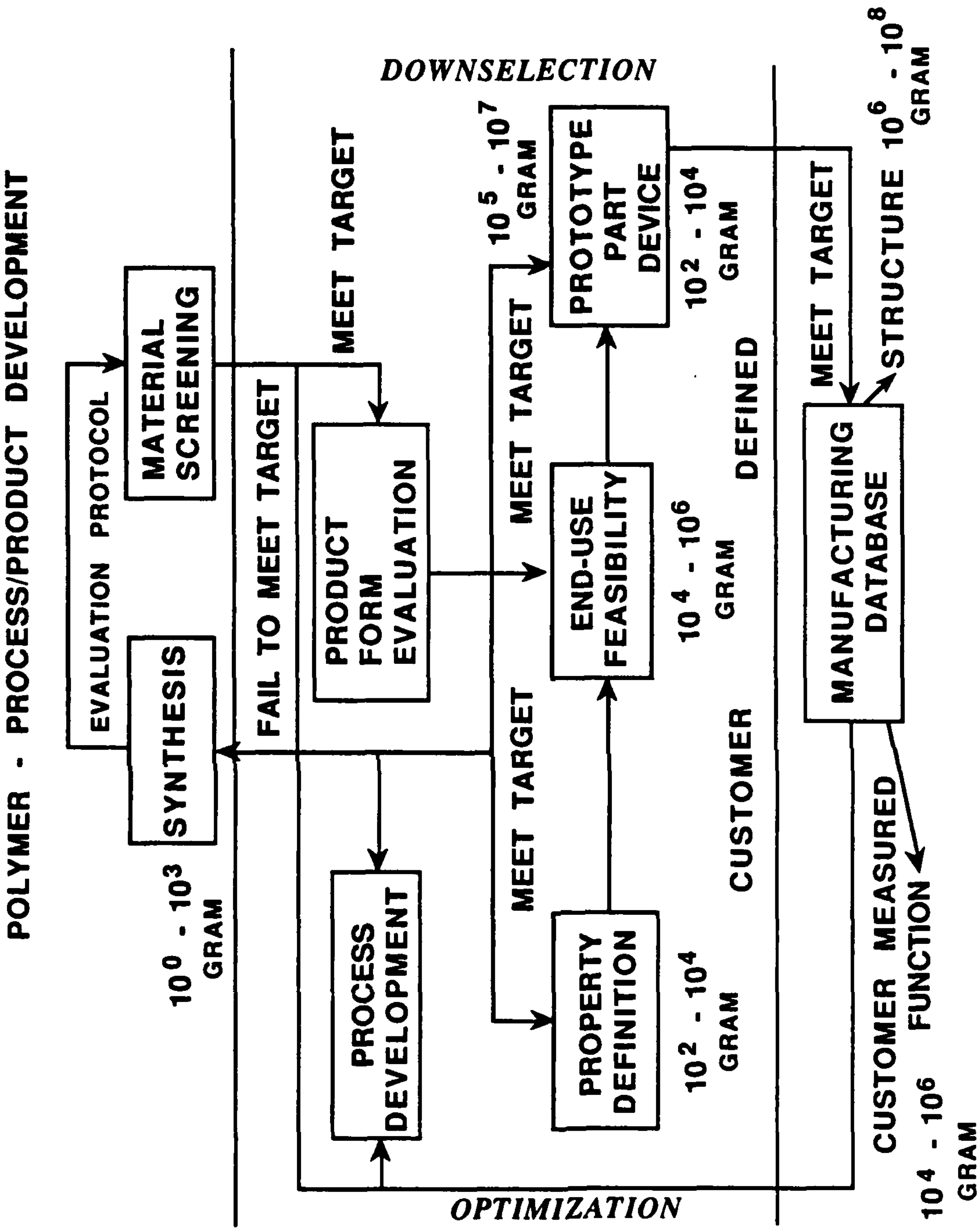


Figure 7. Representation of the iterations and the production scales needed to develop new polymer products and processes (after M. Jaffe).

RESEARCH

The discovery, verification and codification of these critical manufacturing metrics will require new modes of research and the research paths and goals must be formulated differently than was typical in past manufacturing research which were based on comparative studies or focussed on one technology. The proposed research should include features such as:

a. requirement of multi-disciplinary team;
b. hypotheses established in micro-factories (prototyping of metrics):
c. verified in actual plants represented by different industrial environments (technology, market, culture, etc.);
d. improved metrics through iteration and an industry-university-government partnership;
e. statements, equations and relationships which are clear, simple and unambiguous;
f. methods which lead to the discovery and expressions for the interrelationships of the measures; and
g. methods which lead to comparitors which reflect a global or multi-national environment.

The old adage that, "you get what you measure", does in fact emphasize the need to bring a rigorous, science-type approach to the new metrics of WCM. Leading firms use different metrics than their competitors but these metrics appear to be more a belief-set or the mind-set of senior managers. To impact the U.S. industrial base, clear, simple and unambiguous metrics are required to measure the capability and vitality of product realization and drive the appropriate use of and implementation of technology.

VII. AGENDA AND LIST OF WORKSHOP PARTICIPANTS

AGENDA
FUNDAMENTALS OF MANUFACTURING: ADVANCED MATERIALS & COMPONENTS
July 11-12, 1989

Organizers: K. Bowen, R. Mehrabian, K. Adams and J. Williams

Tuesday, July 11

Presentation of Workshop Theme, Format and Desired Output
Introductions: One minute introduction of each workshop participant

Session 1A: Known Rules of Manufacturing
Cook, Elliott, Backman, Pfahl, Wang

Session 1B: Known Rules of Manufacturing
Verleur, Francis, Jaffe, Mar, Moore, Seelig, Adcock, Dowd, Yanus

Session 1C: Known Rules of Manufacturing
Wadley, Parrish

Instructions for Session II: Four Working Groups

Session II: Breakout into four groups which will independently develop lists of most important manufacturing rules.

Conclusion of first day (Chairs of Breakout Groups will meet for one hour to prepare reports of 8:00 AM meeting on July 12)

Wednesday, July 12

Session III: Presentations by chairs of four groups
Known Rules of Manufacturing

Session IV: "Rebutal" Presentations from any workshop participant

Session V: Construct four new groups to re-cast rules
"Generic Rules of Manufacturing."

Session VI: Construct four groups to independently generate list of critical research needs

Session VII: Presentations from four groups
Generic Rules

Session VIII: Looking Forward: What must be done

Session IX: Workshop Summary
Final statement from workshop participants; Statement form organizers
Follow-up Plans

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IX. APPENDICES

APPENDIX A

BACKGROUND : THE CHANGING PARADIGM FOR BUSINESS SUCCESS IN ADVANCE MATERIALS AND COMPONENTS MANUFACTURING

H. K. Bowen, K. B. Clark, B. D. Barnett

The development and use of natural and man-made materials progressed rather slowly until the science and technology of metals, refractories, and glass burst forth in the mid-eighteen hundreds and continued its infancy through the first decades of the Twentieth Century. Indeed, the growth of industrial scientific research occurred in industries like electricity, electric power production, chemicals and communications, where the development of man-made materials played a decisive role. These developments focused on improvement in properties and fabrication processes as well as the development of new compositions of matter. From the discipline of metal physics, which emerged in the 1930's, and the scientific activities in ceramics, polymers, and electronic materials that blossomed in the Forties and Fifties, a science and engineering base was established, enabling advanced materials and components to be fabricated, often for specific end-user applications. The molecular engineering of crystals, for example, has its roots in von Hippel's studies of dielectric materials at MIT, which began in the 1930's. In concert with the emergence of new understanding of the structure and properties of materials, the growth of new industries led to demands for a broader set of materials to meet end-user applications. These demands, in turn, have required an increased understanding of the composition of matter and also of new and difficult processes.

From the late Fifties to the present, the knowledge base for materials and components has exploded. The scientific and technological field of materials science and engineering (MSE) has evolved from a collection of discrete, disparate arts and crafts whose practitioners generally did not stray form their own specialties, to a more integrated character, such that the fundamental knowledge about one materials class is often transferred to other classes. A prime example of the resulting benefit is the extensive knowledge base that has been built in metals solidification rates of alloy systems and the particular equilibrium thermodynamic relationships of a system and its various kinetic coefficients. This knowledge is directly applicable to the solidification-rate behavior of molten ceramic alloys, whose equilibrium thermodynamic and kinetic relationships have similar relative parameters and functional forms to those of the metal alloys.

The growth of knowledge in materials science and engineering and the changing markets and customer requirements in material-using industries has changed fundamentally the demands placed upon firms in the advanced materials business. Contrast the situations facing advanced materials firms today with conditions in the era of bulk materials. In that environment, success depended upon large-scale, high-volume production of a widely used commodity material, where meeting shipment targets, reducing cost, and managing large capital assets was key to success. Meeting delivery requirements, reducing cost, and managing capital assets remain important in today's environment, but the challenges run deeper. Advanced materials firms must deal with a much broader range of customer demands, the levels of performance in the product demanded by customers are much higher and more specialized, the firms must respond to a changing set of demands more flexibly

and faster than ever before, and the critical resources are less physical capital, and more the knowledge of customers, products, materials, and processes. This changing environment in components may be quite different in comparison to the 1950's. The challenge today is to achieve excellence in all of the activities involved in the design, development, production, and distribution to customers. Moreover, excellent capabilities in a functional area must be integrated with other capabilities in the firm in order to achieve superior overall performance. The critical functions in an advanced materials company include 1) the acquisition and implementation of science and technology for advanced material products and processes; 2) a complete understanding of customer needs and, more broadly, emerging markets;
3) superior production capabilities, including product and process design and their implementation; and 4) effective organizations and systems for sales, service, and distribution. The changes in the paradigm to be emphasized here are the requirement for excellence in all facets of corporate enterprise and the assets now required for success. A focus on physical assets (the basis for advantage in the era of bulk materials) must yield to a new era in which knowledge, people, and flexible physical assets combine to yield strategic advantages when used for manufacturing excellence.

Today, advanced materials and components businesses reflect the importance of technology, economics, and organizational structure; it is important to note that local geographic or national conditions may strongly bias any of these. For example, energy costs and local political decisions governing employment currently dominate decisions for locating primary aluminum smelters in newly industrialized countries having energy capabilities and access to bauxite. The macro-economics of such factors as energy and

national policy currently preclude construction of new aluminum smelters in the U.S. It is our contention, however, that many decisions as to which firms are successful in advanced materials and components and where they are located reflect not overwhelming macro-economic conditions, but rather a firm's capabilities at practicing manufacturing excellence in a knowledge-driven environment.

We would like to identify some issues underlying the emerging paradigm for success in advanced materials and components manufacturing. Five key issues concern technology and its implementation, markets, and organizations.

MSE Knowledge

The understanding of materials and the practice of that understanding (MSE) have changed dramatically over the last 30 years. In many ways, the changes have been led by U.S. research universities and corporate R&D laboratories. The most significant step function change to MSE was the creation by DARPA of multiple interdisciplinary materials laboratories in the early 1960's. Significantly, the generation and codification of this knowledge and the training of many scientists and engineers in U.S. universities have resulted in the establishment of numerous groups possessing both the talent and physical facilities to do world-class R&D in MSE. No longer are the critical masses of people and facilities located within few universities or corporate research laboratories; rather, they are distributed among large and small firms, famous and not-so-famous universities, and national laboratories in the U.S., industrialized Europe, and industrialized countries in the Far East. Special tools, instruments, and machines can be purchased by any organization. The number of scholarly MSE journals has risen from a half dozen in the 1950's to

hundreds. Textbooks and monographs have multiplied also, facilitated by the fact that English has become the universal language of science and engineering.

Intrinsic Value of Patents

The explosion of MSE knowledge and the growth of critical mass MSE groups in numerous locations throughout the world has changed in an essential way the role of patent, particularly a composition-of-matter patent, is likely to confer less of a dominant advantage than in the past. At the root of this change is the growth in the number of alternative routes to achievement of a given performance objective. With the growth of understanding of the relationship between structure, properties and performance, scientists have developed the ability to achieve similar levels of performance with a variety of compositions of matter. At the same time, customer demands for specific and peculiar performance with a different composition of matter, thus reducing the potential for dominance in the market. In addition, it is unlikely that the firm will be able to develop and patent all of the relevant compositions for all of the relevant applications. Thus, incentives exist to use patents to establish relationships among competitors, to license and pursue joint ventures and to engage in technology exchange agreements that preserve the firm's ability to compete in a wide range of applications. Those patents remain important, but their role today is not to confer dominance in the market, but to allow the firm to participate in the game.

Time-to-Breakeven

Advanced materials play a crucial role in downstream systems. In advanced computer systems, for example, system performance is heavily

influenced by developments in materials for packaging IC ships as well as the chips. The material is thus an integral part of the design and development of the system. It is not specified at the end after systems requirements have been established and the design has been accomplished. Rather, it is an essential part of the early phase of development. The central role of advanced materials creates both a significant opportunity and a significant challenge. On the one hand, its central role in the system means that it creates opportunities for value added through materials development. The challenge is that advanced materials producers not only must be capable of production in volume at high quality, but also must participate in prototype development and in the qualification cycles that exist in complex system developments. End users of advanced materials and components demand new material compositions and new forms in prototype as well as full production quantities. This requires the invention of both new materials (composition, structure, form) and new processes (physio-chemical parameters, machines, systems, and so forth). Furthermore, all of this activity may take place several years before significant revenues and profits are generated. In this context, having material science capability, even to the extent of creating an exciting new material, is unlikely to be sufficient for success. The challenge is to be able to participate in the development process, to be credible to potential customers, and to do all of this with short turnaround times and at low cost. The challenge is thus to operate innovatively, rapidly and efficiently in order to reduce substantially the time to break even. Time to break even is the time required to take a concept from research to production and to produce enough revenues that profits equal the costs incurred from the beginning of the R&D phase through start-up and production. Time to break even is likely to be a critical determinant of success

in future advanced materials markets. It is determined not only by the eventual margins on the products, but also by the time, efficiency, and responsiveness in the development process.

Proliferation of Products

As a result of both the seemingly limitless options offered by MSE and customers' insatiable wants, the advanced materials and components business has produced a plethora of products differentiated not only by composition of matter (e.g., various metal alloys) and material class (e.g., metals and polymers), but also by shape, form, and structure. The customer has demanded that producers move from a few types of steel to hundreds of steel alloys and from a few polymers to hundreds of compositions and blends. A corollary seems to be that the more value added during fabrication, the more severe the differentiation in composition or form, oftentimes leading to composite structures. For example, the most sophisticated packages of VLSI ships are made from metals, ceramics, and polymers in interpenetrating layers -- all requiring sophisticated processing to create particular micro- and macro-structural features to produce the desired performance characteristics. The proliferation and differentiation of products are driving the advanced materials and components business to a very large number of small-volume markets in which knowledge, flexibility, and time are critically important. In earlier eras of new materials developments, markets and volumes could not be predicted accurately and niche strategies were often the required entry strategies. Today, it appears that there will be very few additional high-volume products like iron, steel, nylon, polyethylene, silicon, and alumina. The global marketplace and the other issues described in this document appear to intensify the need to

identify a clear market entry strategy may be an important key to pulling technology into the marketplace.

Design-Manufacturing Integration

Concurrent engineering, or design-manufacturing integration, is more important in the new paradigm than in that of the past. Though this fact could be considered a subset of the time and product proliferation issues, it is discussed separately here because of the new knowledge and mind-set required of the practitioners of advanced materials and components manufacturing excellence. Some of the most compelling successes in the area of advanced materials and components recently have been those in which the processing knowledge base allowed the community to establish "producibility rules". Extensive knowledge about production processes, machines and systems were translated into design rules for producing the product. For example, the designers of VLSI chips or optical wave-guide components have clearly stated and documented rules for the composition, shape, proximity, etc., of various combinations of materials that go into the final product. These rules, when practiced, essentially guarantee that the designed device can be fabricated. It should be recognized that the quality and production yields of these advanced materials and components depend on many other features of the organization and its knowledge and practice of manufacturing excellence; "producibility rules", however, are critical. This is one aspect of concurrent design; other aspects include the detailed data on properties, performance, end-use environment, etc., and the mathematically (statistically) based models and simulations to design both product and process.

Summary

The new paradigm for success requires new knowledge and methodologies of manufacturing excellence yet to be discovered, and the environment and forces at work make a strategic advantage difficult to maintain. Why, then, would any firm be interested in entering the advanced materials and components manufacturing business? There are several reasons. The first has to do with the notion of value added: although the elements of manufacturing excellence required to successfully participate in these markets have yet to be established through research and practice, it is clear that profits to those who successfully participate are much larger than the margins associated with materials markets of the past, for example, Kyocera, with $2 billion in annual sales, now has a $1 billion cash reserve. Second, it is clear when one tracks either the growth rate of new materials markets or the displacement of old materials and components that many of the old markets do not offer satisfactory business opportunities for the long term. For example, aluminum producers must continue to evolve products through innovations in alloys and processes. Third, though past business offered simple substitutes of one material (e.g., with a higher specific modulus for another, the driver for advanced materials and components market growth is largely the performance of new systems incorporating the substitute products: optical wave guides, for example, are much more than just replacements for copper in telecommunications. The consequence of these and other factors is that many firms in Western Europe, industrialized nations of the Pacific Rim, and the U.S. have recognized that advanced materials and components represent one of three key technologies expected to lead innovations for productivity and competitiveness in the Twenty-First Century; the others are biotechnology and information technology. Identification of these by companies and national commissions has resulted in

the establishment of national commissions has resulted in the establishment of national strategies. The strategies and resources available in several European nations and Japan appear especially effective, and geared toward resolving many issues in advanced materials and components manufacturing now perceived as problems.

APPENDIX B

ADVANCED MANUFACTURING PROCESSES WHERE CRITICAL INNOVATIONS ARE STILL REQUIRED

J. Economy

One of the recurring problems in establishing an advanced manufacturing line in highly competitive industries is the urgency to define the process even though one or more of the critical components still require significant innovation. This kind of phenomena is so common in some industries that the organization becomes geared to operating in a crisis mode. Obviously, the amount of waste is great and the actual cost to bring a process into manufacturing is enormous. Clearly, patterns (or rules) for functioning in a cost effective way in such an environment would be extremely useful. Furthermore, successful implementation of such rules over a broad range of U.S. industry would permit for a major advance over current practices in countries such as Japan. In other words, the key would be to exploit the unique innovative skills of the U.S. technologists along with the very clever techniques in automation now being practiced in Japan to accelerate commercialization of new technology in a cost effective way.

There are, of course, many examples to draw from to illustrate the tremendous cost associated with establishing manufacturing lines where critical components where or are still lacking. These include the aramids, multi-layered ceramics substrates and currently the 16M bit DRAM chip.

Generally the primary problem is that these programs are driven by manufacturing engineers who are not skilled in the process of innovation. An

extreme example of this problem is illustrated from the following narrative describing the development of Kynol, a flame resistant phenolic fiber.

In 1969 the Carborundum Company announced the commercial availability of this fiber. Up to that point a rather crude, very expensive 15 step process had been designed by Research for preparing the fiber as an uncrimped staple that was non-uniform in length and diameter. The New Products Group assigned to this project proceeded to scale-up this process in order to provide customers with samples of the new fiber. Obviously, the impact of this product on the market place was at best marginal. In 1972 the activity was reorganized so that the research, marketing, engineering and manufacturing were placed under a research manager. Within one year the process was reduced from 15 steps to three yielding a uniform, crimped fiber which was readily processible on standard textile equipment. Furthermore, the cost was cut from $15/lb to $2/lb with the *potential of getting down* to under $1/lb in a multi-million pound facility. This example indicates the importance of the R&D function in establishing a manufacturing line when key technologies were still missing.

A somewhat different example is afforded by the activities of the polymer research activities in IBM. During the past decade a number of research programs were initiated on advanced polymers which might find use in advanced devices which were still on the drawing board. These activities were aimed at designing new polymers which solved at least several of the key materials properties that might be required for use in the advanced device. In fact, with such an approach it invariably turned out that once materials requirements were defined for a specific device, it was possible to tailor the new polymer to the need and to provide manufacturing quantities within 2-3 years

after the request was made. To generalize, in those industries where rapid technological change is occurring, it is essential that small groups of materials scientists carry out the longer range research designing new materials which can then be tailored to the specific use that emerges.

APPENDIX C

JAPAN'S MANUFACTURING PLANS

The planning documents of firms or nations seldom are the actual paths of evolution. However, the planning documents from Japan do give insight to strategies which are often put into motion. The recently translated document of the Japanese Machinery Federation Plans for the evolution of manufacturing systems is captured in this appendix in a very brief form[1]. The analysis and plans call for clear and aggressive responses to the changing of political and economic conditions based on redefining the rules of manufacturing for strategic advantage. The new Japanese manufacturing paradigm may again displace U.S. firms in their attempts to achieve the old paradigm.

From the DoD perspective of a industrial base for ship building and aerospace, the Figures C-1 and C-2 are instructive. A national agenda is proposed for Japanese companies to become competitive in these two segments, using their established capabilities with new intellectual assets acquired from a broad until their own research puts them in a leadership position.

Characteristics of Japanese Manufacturing systems and Their Competitive Advantage (Directly from the Japanese Document)[1]:

"This section will provide an overview of the manufacturing systems that have made Japan one of the leading industrialized countries, and the factors that have made this possible.

It is thought that the "Pax American" has been the foundation of our economy and society. The fact is that the United States has been the economic leader and has developed a market that absorbs manufactured goods, and had a strong currency which stabilized the currency markets, promoted worldwide

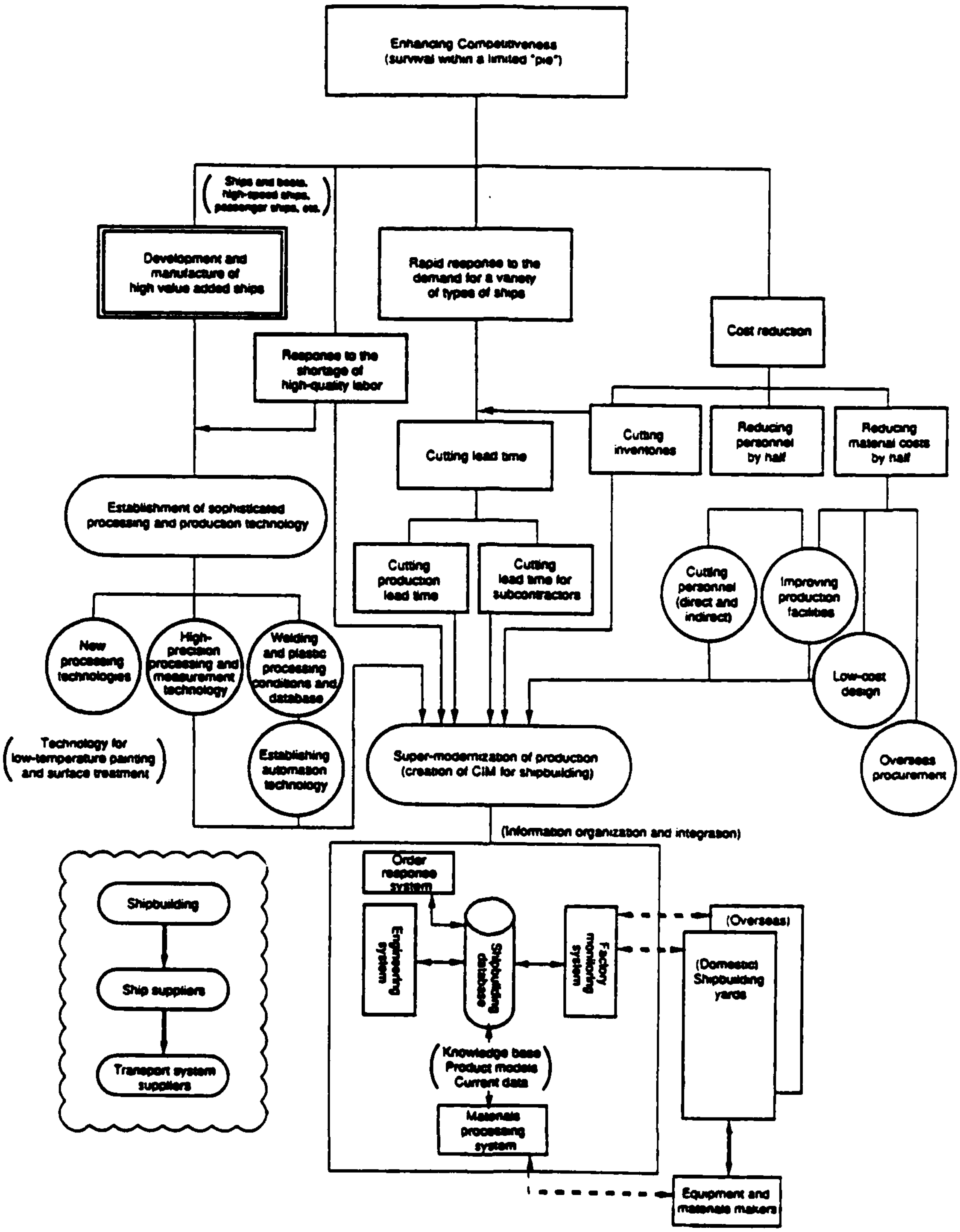


Figure C-1. Future Tasks for Japan and Manufacturing Systems Trends in the Ship Building Industry.

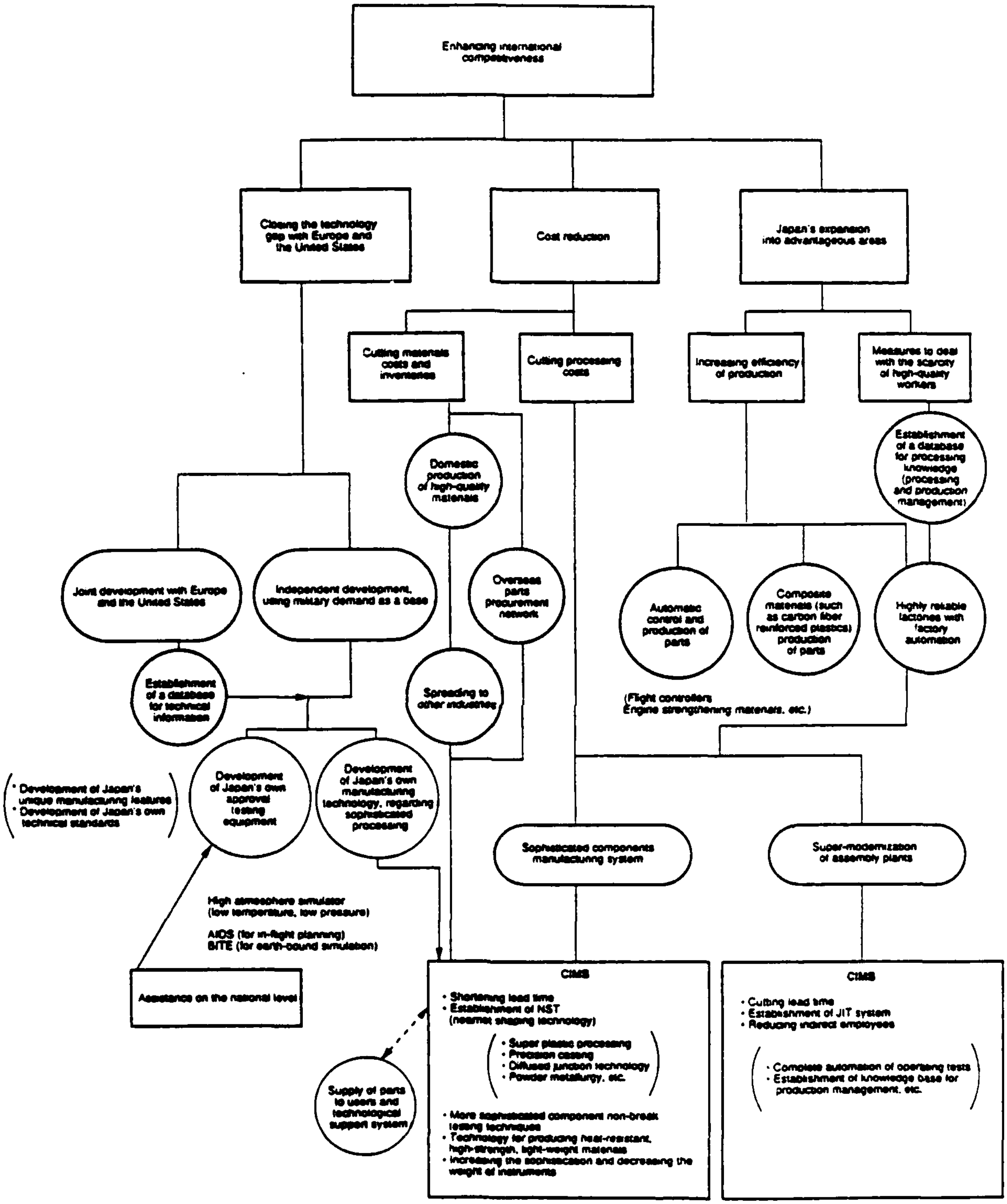


Figure C-2. Future Tasks for Japan and Manufacturing Systems Trends in the Aerospace Industry.

economic activity, and made possible the development of enterprises in Japan and the NICs, due to their dependence on exports.

Higher economic growth has been supported by receptive foreign and domestic markets and by large-scale investment that shows confidence in future economic growth, and the competitiveness of enterprises has increased. In the case of Japan especially, it cannot be overlooked that the high savings rate of the Japanese people has produced a financial market that is favorable to future investment.

Education and the educational system, which provide an essential base for industrial expansion and growth, have been advanced in a direction that strengthen industry. This ensures a high quantity and quality of labor, and has made it possible to ensure the homogeneity of the labor, and has made it possible to ensure the homogeneity of the labor force, which is most essential for organizational cohesion in fields such as manufacturing. (This has been a large factor in the development of domestic industry overseas).

Even when we look at technology, we see that there have been no innovations in the past few decades that have called for great break-throughs, and products and manufacturing technologies have developed almost continuously. Thus, the development of markets, products, and technologies, rather than developing intermittently, have progressed steadily.

In the past, the two oil crises, pollution, environmental problems, and problems with natural resources have dealt blows to the development of manufacturing, but these problems have been overcome for the mid-term, and are thought to have almost stabilized."

The strength of Japanese manufacturing resides in macro-level (national) policies as well as micro-level (company) strategies and with systems for hardware and infrastructure. In the recent past these have been[1]:

"National Policies: Priority production policies, protection of manufacturing, training, and other economic and industrial growth policies have long been supported by strong leadership.

Socioeconomic Environment: A great deal of effort has been devoted to the promotion of education and training of technicians for the sake of cultivating manufacturing personnel. Workers have come to feel a sense of fulfillment in their work, and place a high value on the "sweat of their brows." Furthermore, Japanese employees in manufacturing (including sales personnel) speak the same language and are of the same race.

Manufacturing Capacity: High growth and the healthy desire for investment which is supported by favorable financial markets have greatly enhanced manufacturing capacity (quality, productivity, and cost). This has also had a positive effect on the acquisition of new technologies, including on-site know-how. This has primarily been a domestic phenomenon, resulting in a manufacturing system (manufacturing network) that includes orders to outside manufacturers, subcontracting, and purchasing.

Management Systems: While businesses in advanced countries such as the United States and European countries have emphasized marketing and financial manipulation in their management policies, Japanese manufacturing enterprises have given priority to manufacturing in the broadest sense, including both production and technology. Japanese companies have also achieved a competitive advantage by utilizing a Human Resources Management System; a complex that includes life-time employment, a seniority system, intra-company labor unions, and paternalistic management practices that is suited for enhancing manufacturing efficiency in a high-growth environment. Such a management system involves a manufacturing network

whose members share a common fate, and has an approach to systems improvement which includes company-wide TQC, quality control circle activities, and the just-in-time (JIT) system, which back up the Human Resource Management System. This latter approach is known as the "small steps" approach, and involves a realistic step-by-step trial-and-error method. This approach is adapted to the conventional manufacturing environment of mature production, repetitive production, and mass-production.

The Environment for Manufacturing in the 21st Century

"Generally speaking, in the case of mature production, the development of markets and technologies is not intermittent, but rather is continuous, and advances almost as predicted, building on past achievements, Given such an environment, competitiveness will be based on the convergence of the energies of all employees, and on the steady accumulation of small improvements. This trend is especially strong in the manufacturing industries. Taking these points into consideration, the industry in Japan that has especially strong international competitiveness is the electrical machinery industry, which has a mature product line that can be mass produced repeatedly, and is suited for assembly.

However, the strength of Japanese enterprises does not come from their ability to succeed under any type of conditions, but from an environment in which competitive advantage arises and from the presence of competitive elements that respond to that environment. Thus, the question is, what changes will take place in the factors that give rise to competitive advantage in the future, and what reforms must be made in competitive factors so as to bring out competitive advantages that are responsive to these changes?

The most noteworthy environmental change is the shakiness of the "pax Americana." However, we don't expect another country to replace the United States as the leader of the world at least until the beginning of the 21st Century. Thus, for the time being, all we can hope for is a "Pax Consortis," in other words, a joint management system resulting from the cooperation and solidarity of the developed countries. Such an arrangement will result in a greater burden of responsibility on the shoulders of Japan, and will repeatedly draw Japan into activities which are limited by the requirements of international harmony.

The decline of the "Pax Americana" will probably give rise to unstable currency markets, increases in the gap between politics and economics, increased trade frictions, and international "me-ism" such as economic nationalism. The economy and markets will most likely mature to a greater extent. In addition, the Asian NICs will make dramatic progress from their status as "middle class" countries. This means an increase, and these information resources will be directly linked to management strategy in a more intimate way than other management resources.

Until now, the development of technology has occurred somewhat continuously, but in the 21st Century, it is highly probable that new technologies will be developed by means of a heterogeneous combination of conventional technologies and biotechnology, microelectronics, and new materials. In this sense, technological innovations will be more intermittent than in the past.

In addition to the development of an "informatized society" and "globalization," we expect that socio-economic maturity will bring about changes in the way people think as well as changes in their values. In the past, the sphere of activity tended to be group oriented, but we think that in the future, more individualistic ways of thinking and value systems will come to the fore.

Our above discussion has presented an overall view of the environment for Japanese business as it approaches the 21st century. Of course, changes in these environmental factors will affect the competitiveness of these businesses. The question is: what changes will take place in the factors that have influenced the competitive advantages of Japanese enterprises in the past, and how should we respond to these changes?

For a long time, the Government has taken the lead in promoting education and growth in business, and has provided support for business, but we think that in the future, unified public and private policies may be difficult to implement. On the contrary, taking a point of view that looks beyond Japan, it will probably become necessary to implement regulations and restrictions on the free activities of enterprises. Moreover, with the rise of individualism and advances in the globalization of enterprises in the future, it will become impossible to utilize a management system that assumes a homogeneous workforce that is the the same race, as in the past. In some cases, the strengths of the past may become weaknesses in the future.

The maturation of industry and the economy tends to place greater emphasis on financial and marketing functions in manufacturing industries, as well as on a shift in the workforce from secondary industries to tertiary industries. This will cause a decline in technical and manufacturing oriented education. In fact, signs of this have already begun to be seen. The "softening" of the economy has brought about a shift from physical labor to knowledge-oriented work. There will most likely be a great change in the accompanying attitude towards work. There may no longer be the sense of fulfillment in sweating for the sake of the company.

Changes in the external environment will probably also bring about a decline in the desire for investment, which was so prevalent in the past. Investment decisions will be made more carefully, and the risks will be greater. New technological innovations, including combinations of technologies, will bring about a need for breakthroughs. The emphasis on information resources as one type of management resource will require changes in Japan's industry, which has heretofore been in an advantageous position in the area of hardware.

Because of these changes in the business environment and in competitive factors, there will have to be great reforms in management systems. Enterprises have already started to show signs of change in their management strategies in response to these changes in competitive factors. There has been more emphasis on ROI and a larger number of mergers and acquisitions than ever before. Wages are now being based more on ability and efficiency than on seniority as in the past, and instead of the implicit organization and management style, there is now a tendency for Japanese companies to have their management "go by the books" in a clear and explicit manner, as in the United States and Europe. Moreover, company-wide total quality control groups, whose aim was to improve manufacturing systems by using a realistic trial-and-error and step-by-step approach, have gone about as far as they can go, and are now tending to have less effect. It will be difficult to overcome this problem by conventional approaches alone. The movement toward overseas production and "globalization" of enterprises is likely to accelerate in the future. This "globalization" will make it necessary to develop a system that will be valid not only in Japan but throughout the world.

We would now like to summarize the response to changes in competitive factors in the 21st Century.

(1) Metamorphosis from "followership" to leadership, requiring

- A move from technological imitation to technological innovation;
- A developmental and creative organizational system;
- Individualism in enterprises.

(2) Reform of Human Resources Management Systems, requiring

- Reform of the lifetime employment and seniority systems;
- Response to the shift from a homogenec workforce to a heterogeneous workforce;

(3) Reconsideration of means for expanding sales and market share, and responses to lower growth.

(4) The development of and response to global business.

(5) Reconsideration of the merits of scale (large does not necessarily mean advantageous - discovery of the merits of s..iall size).

These issues will have to be considered in the reconstruction of manufacturing systems as we face the 21st Century. For example,

- Shall we replace the paradigm of large-scale mass production with a new paradigm (small is beautiful)?
- How shall we utilize the efficiency of indirect work (hidden factories) given the greater demand for knowledge over the traditional labor?
- What kind of system should we establish to develop a global business?

- Assuming that we can no longer maintain the conventional human resource management, what type of system should we develop?

There are many other issues as well. The world has given Japan the task of developing manufacturing enterprises and manufacturing systems that harmonize with the rest of the world, whose presence is recognized as necessary by other countries, and which are competitive."

DARPA INITIATIVE TO ESTABLISH A U.S. BASE FOR MULTI-CHIP MODULE SUBSTRATES

H. K. Bowen, B. Gilbert, J. Murphy and R. Mehrabian

Electronic systems are only as good as each of the components and subsystems. While semiconductor chips receive the most attention, the interconnection or packaging technology is equally important to systems performance, reliability and cost.

The microelectronics packaging market consists of many segments. The largest number of packages are low lead count, plastic packages. The most sophisticated incorporate features of very high I/O interconnects (chip to package), hermeticity, and materials and design compatibility to high heat dissipation and to minimum mechanical stresses. The future high performance packaged systems will rely heavily on multichip and hybrid configurations where chip packing density and manufacturing compatibility will be the key additional drivers.

The dilemma for the DOD and the U.S. electronics industry is that there are no notable and credible merchant suppliers of the multichip substrates. Demand for the completed modules (chips installed on substrates) is expected to have a compounded annual growth rate >100% and be many billions of dollars by 1995. The MCM substrate business will have a similar growth rate to become $300-400M per annum by 1995. In the near term, these MCM substrates are likely to be a combination of a multilayer ceramic substrate and a multilayer thin film metal (copper) and polymer (polyimide) overlays.

The MCM technology was pioneered by IBM, which has made huge technology and production capacity investments, but for internal use only. The firms most likely to introduce MCM technology are Japanese: Fujitisu (which has announced a computer system using it), NEC, Hitachi and Kyocera. What is potentially devastating to the U.S. commercial semiconductor producers (TI, Motorola, Intel, etc.) the commercial systems houses (DEC, HP, Sun, etc.) and the military system houses (E-Systems, TRW, Hughes, Northrop, Lockheed, etc.) is the coupling of Japanese MCM technology with Japanese merchant chip production capabilities (volume IC's and ASIC). Thus; success in MCM substrate production can be used strategically to dominate the subsystems (high value-added) markets and upset the strategic plans of a significant number of American electronics manufacturers.

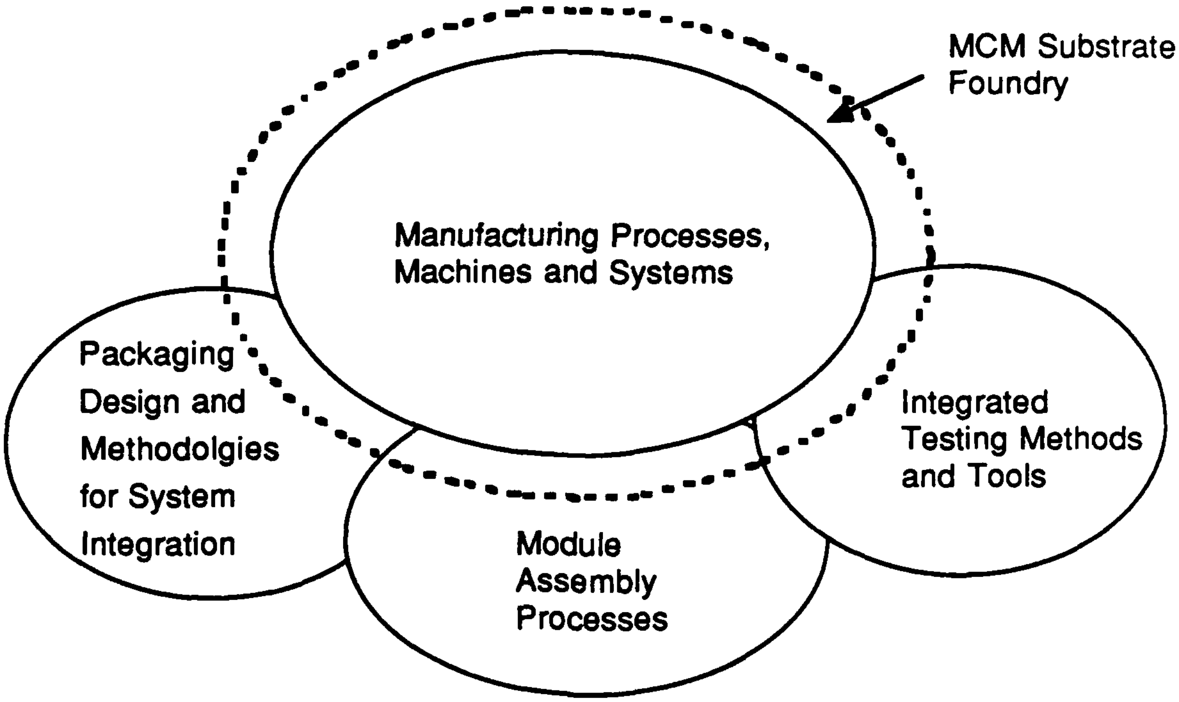
It is proposed that DARPA take a leadership role in establishing MCM substrate manufacturing technology. Two pilot line foundries should be established and run in such a way as to understand and implement world class manufacturing principles. The pilot lines should be focused on the production of first generation products for insertion into prototypes systems in late 1991. Each MCM foundry should deliver to a DOD customer and a commercial customer (e.g., a military signal processor and an advanced workstation). The experience from these pilot line foundries will provide the underpinning to determine whether to establish a major production company, U.S. MCM Substrates, Inc. in a second phase of the project.

The criteria for defining DARPA's program, and thus for defining the MCM substrate products and production processes and for selecting the firms to build and run the pilot line foundries, are as follows:

1. Technology Pull - identifiable customers, products and systems for the initial substrate production;
2. Dual Use Production Systems - products can be customized for a military insertion and for a commercial system;
3. Investment leads to Multiple Merchant Suppliers of MCM Substrates - meets the requirement that there be multiple sources for key components; and
4. Solves the Infrastructure Problems - recognizes that people must be developed (i.e, trained) in addition to generic processes and production systems.

The key recommendations are for two commercially driven pilot lines and for two companion university based manufacturing programs oriented to the preparation of students in the required multi-disciplinary manufacturing technology. The university efforts would mimic in a research sense what is being developed in the commercial setting, but be focused on training and education of people (especially engineers and technicians) in the manufacturing principles (design, production, machine design, etc.). Thus, the DARPA program centers on the pilot-line concept, i.e, on a series of steps resulting in the creation of an MCM Substrate Foundry, a place where systems builders (module designers and users) can bring problems and achieve solutions leading to tangible manufactured products.

The knowledge resources and the technologies which will be the foundation for the pilot-line foundries are shown schematically below:



The capabilities in each of the four arenas are shown by the circles. Each pilot-line foundry would require the capabilities shown by the dashed line; that is, it would not be a module assembly house but it would have machines and people of sufficient breadth and sophistication to solve assembly problems (e.g., understanding of wire bonding, TAB, or flip-chip attachment technologies, and hermetic encapsulation) for the system houses who will use the substrates. Issues associated with the packaging of high density, moderate speed integrated circuits (clock rates under 100 MHz)and the encapsulation of very high clock rate systems (greater than 250 MHZ) should be addressed by both of these foundries.

The two university programs should develop people and knowledge to support the principles encompassed within the dashed line. The university

programs would require a multidisciplinary approach (engineering disciplines and management) and perhaps a heavy emphasis on masters-level students who will serve as the next cadre of sophisticated manufacturing staff for the foundries and for the end users (i.e., the systems houses). Much of a student's thesis research may (should) be conducted at industrial sites on production or pre-production equipment.

To accomplish the development of a U.S. MCM substrate industrial base, a phased program with a five year total commitment will be required. By the fourth year, the data would be available for a decision as to whether DARPA should lead in the establishment of a major new firm supported by end users. The companies operating the pilot-line foundries would be free to let the market pull grow their stand-alone commercial enterprise irrespective of the DARPA decision to create the large entity.

The 5 year commitment from DARPA would require funding levels of:

Year	1	2	3	4	5	TOTAL
Per Foundry ($M)	4	8	12	10	7	$41M
Per University ($M)	2	4	5	5	5	$21M

U. S. COMPETITIVENESS IN CERAMICS

H. K. Bowen, E. Cross, A. G. Evans, R. Mehrabian, W. Barker and B. Wilcox

The design and development of advanced ceramic materials and components has been a forte of the American R&D establishment. However, with a few outstanding exceptions, the commercial success of these products has been captured essentially by Japanese firms and it appears that the potential for growing new markets and extending established markets will continue to be dominated by Asian companies (Japan and Korea). Recent examples of U.S. commercial successes have been IBM's multichip package, Corning's catalytic substrate for auto emissions control, and AT&T's and Corning's optical waveguide products. It is also likely that Lanxide Corp. will establish a reasonable U.S. market for ceramic armor within DoD and wear resistant parts for automotive and other commercial applications.

While there are still major merchant suppliers of ceramic-based products in the U.S. (e.g., Corning, Norton, Champion Sparkplug, AVX, Sprague, Coors, Carborundum-BP, etc.), there are major markets not being addressed and the growth of advanced ceramics markets by these companies is much less than comparable Japanese companies. Major merchant suppliers in Japan (Kyocera, TDK, Murata, NGI .1sulator, NGK Sparkplug, etc.) as well as integrated companies which have major merchant-based ceramic divisions (e.g., Matsushita, Hitachi, Toshiba, etc.) bring significant financial and intellectual resources.

Let us define world class manufacturing of advanced ceramics to include key capabilities to (1) introduce new technology, (2) improve current advanced products (productivity), and (3) grow new businesses. In short world class

ceramics manufacturers have long term profits and growth by responding to customers needs. With this view one can give a harsh assessment of the results of efforts by major U.S. companies to be WCM in two particular market segments: advanced structural components and electroceramics.

MAJOR U.S. COMPANIES WHICH HAVE TRIED BUT ARE NOT WORLD CLASS MANUFACTURERS.

Advanced Structural Ceramics

Ford	Westinghouse	Air Products
Norton	Dow Corning	W. R. Grace
Dow Chemical	Celanese	Carborundum (BP)
Alcoa	Garrett/Allied Signal	AVCO (Textron)
G.E.	G.T.E.	Corning
PPG	Coors	

Electroceramics (packages, capacitors, etc.)

3M	Augat	Union Carbide
G.E.	Sprague	Western Electric (AT&T)
O.I.	Raytheon	San Fernando Electric
Cabot	W. R. Grace	Dupont ?
Coors	GTE	Ray Chem ?
Corning		

There are many reasons why these companies have not succeeded. The simple description would state that issue it is due to a lack of long term commitment of resources because of WallStreet's financial return requirements.

However, since many of the major Japanese competitors are also very profitable (e.g., Kyocera with $1 B cash reserve), one must look more deeply. The U.S. ceramics firms have not practiced principles for world class manufacturing; specifically, on average they have:

(1) Minimal design capability and especially process driven design rules to interface with customers;

(2) Ineffective and inefficient technology implementation processes to take advantage of their own and other's research and development results;

(3) Insufficient investment in the knowledge of processes and manufacturing systems: the hardware, software, humanware, etc; improvements and future developments;

(4) *Failed to develop commercial processes which are* flexible (material composition and component shape tolerant) to respond to the product proliferation and small volume requirements; and

(5) Failed to develop technology (processes, machines, systems, etc.) which attack the fundamental barriers of cost, yield, timelines, rapid prototyping, etc.; and

(6) Not established the critical mass of key people and technologies to service customers and not developed the customer base to let the market pull their technology based products.

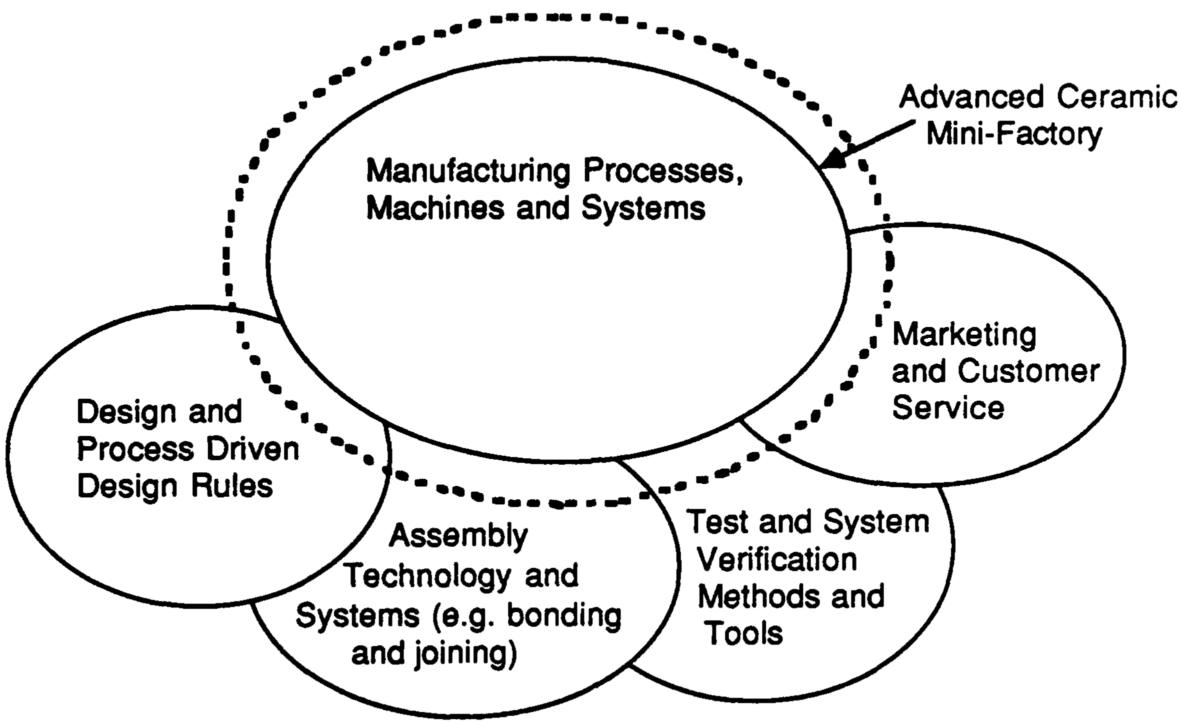
What has changed? The most significant feature is the customer base, the market pull structure, wants U.S. manufacturers. It has finally been

recognized by integrated manufacturers and assemblers (autos, capital equipment builders, electronic systems houses, etc.) that advanced ceramics are critical elements in their systems. This recognition would enable a DARPA initiative to realistically affect the industrial base by assuring that the results of DARPA programs are broadly used and are factored into design and fabrication actual systems (military and commercial).

It is proposed that DARPA establish a minimum of four demonstration factories (mini-factories or pilot-line foundries) to understand and thereby demonstrate the principles for world class manufacturing. Each foundry should focus on the integration of knowledge and known materials and technologies and understanding the product realization system. This initiative should not seek to invent new materials, new sensors, etc. The operation of the system to understand world class manufacturing, to create the new manufacturing metrics and to develop process driven design rules is the most important function of the DARPA program; although a significant by product will be U.S. production capabilities which meet world class standards.

Because the workforce (engineers, managers and technicians) is equally important to success of a manufacturing enterprise as is technology, it is proposed that there be a university "factory-oriented" program associated with each foundry. The university program should develop a cadre of people capable of working in such a company and be responsible for the more fundamental research on manufacturing principles. The university programs must be multi-disciplinary and encompass the disciplines required in the advanced ceramics product realization business.

A method for understanding the concept for the four pilot line foundries or mini-factories is to consider the knowledge required to be successful:



Each DARPA funded entity is to drive to early commercialization of an advanced ceramic product for dual use - military and industrial. Each will have adjunct intellectual resources from the companion university program and the other knowledge sources, especially it's customers. Each foundry must have the critical mass, (knowledge bases) but the major expenditures should be for the manufacturing system to produce real products. CAD tools, for example, will need to be acquired from other sources and not developed by DARPA in this program. Although each foundry should allow for initial activities in concurrent engineering (product design compatible to its manufacturing processes). The mini-factory should be capable of production levels to 1,000/day to learn from statistically-based analyses and be capable of improvements to the initial production tools, processes, and machines which evolve to optimized systems. The factory experience must provide the foundation for breaking the current cost, yield, and flexibility barriers and verify the metrics for product/process

performance. It should provide the setting for understanding the new dimensions of workforce skill requirements and teaching methods.

The 5 year commitment from DARPA would require funding levels of:

Year	1	2	3	4	5	TOTAL
Per Foundry ($M)	4	8	12	10	7	$41M
Per University ($M)	2	4	5	5	5	$21M

The advanced ceramic products to define the minifactories would be those in which there is currently a market pull (military and commercial sectors) such as:

1. monolithic structural ceramics (e.g., Si_3N_4 bearings)
2. ceramic fiber based composite (e.g., Ti matrix/Al_2O_3 fiber composite, ceramics & fiber reinforced ceramics)
3. multi-chip module substrates
4. ultra thin multilayer dielectrics
5. CVD Coatings (e.g., duplex, engineered coatings to toughen brittle matrix composites)

Finally, the emphasis of the minifactories would be to produce products suitable for insertion in existing DOD applications. A possible approach would be to establish these minifactories in U.S. companies with existing manufacturing capabilities to minimize DARPA investment and exploit available resources; both physical plants and people.

MATHEMATICAL MODELING

A. T. Patera, with J. R. Rice

EXECUTIVE SUMMARY

This one-day meeting was organized by Louis Auslander, Director of the Applied and Computation Mathematics Program (ACMP) in DARPA-DSO. The meeting comprised some brief comments by Auslander, and four one-hour talks by H. Levine (UCSD), S. Boyd (Stanford), J. Derby and G. Sell (U. Minn.), and S. Orszag (Princeton); each presentation involved extensive discussion. The objective of the conference, as in past ACMP appearances at MRC meetings, was to create closer ties between the ACMP program and "client" disciplines and projects at DARPA.

H. Levine's talk focussed on the mathematical modeling and solution of problems involving the early stages of dendrite formation in solidification processes. Levine described a mathematical model for a binary alloy. His model includes a Stefan problem for concentration diffusion with a reasonably realistic interface condition. However, it neglects temperature variation, bulk motion in the fluid phase, and elasticity and stress in the solid. Analysis of the "steady" problem shows that the velocity of the Ivantsov needle is determined by the solution of a singularly perturbed eigenvalue problem and that anisotropy of surface energy is critical to the existence of the solution. Linear perturbation analysis was aimed at predicting the appearance of side-lobes observed in experiments; however, their full explanation remains to be found. Future work will address three-dimensional and nonlinear effects, as well as more realistic

material systems. The extent to which this work is directed towards, or can lead to, the understanding of actual solidification microstructures is not yet certain. The work described by Levine is part of a larger inter-disciplinary effort with contributions from "pure" and applied mathematics, computational science, and materials science. It is clear that the results of the mathematical analysis are singularly dependent on the interface-condition physics, and that iteration between model, analysis and experiment is therefore a prerequisite for success. It is also apparent that there are other (i.e., "competing") mathematical enquiries into dendrite growth in progress (e.g., at Caltech) and that the parties involved might benefit from better communication.

The talk by S. Boyd comprised a general-audience review of control theory and practice, followed by a brief discourse on new controller-design methods currently under development. Boyd described old methods (e.g., PI control of the "closed-loop-at-a-time" variety), new methods (solution of model systems leading to multi-parameter optimization), and "newest" methods (determination of optimal multi-parameter transfer functions - and subsequently control parameters - for a particular system by direct solution of a convex optimization problem). The convex constraints may include, for example, restrictions on the time history of unit-impulse responses, or minimization of r.m.s. spectral error. To the uninitiated, the "newest" control methods appear to be extensions of successful methods used in optimization theory to problems involving uncertainty (and hence *requiring control*). Boyd described the relative utility of these various controller approaches as a function of model-precision and degree-of-control required. Boyd stated that current industrial practice is relatively crude, at least as regards "low-level" linear modeling; high-level, highly nonlinear control strategies were not discussed in the talk. Boyd's basic tenet, perhaps more general than the particular controller-design strategy

espoused, is that the recent dramatic improvements in hardware cost and speed allow for no-cost-increases in controller effectiveness through pre-processing (computationally intensive design of better controllers), and real-time processing (e.g., use of multiple inputs, controller modification).

The joint talk on mathematical modeling and inertial manifolds by J. Derby and G. Sell began with an introduction by J. Derby on the numerous problems in materials processing which can benefit from mathematical modeling. Derby described, in some detail, the modeling of Czochralski growth of semi-conductor crystals, focussing on the dependence of material quality on processing history, and on the ability to understand process history through accurate mathematical modeling and solution techniques. G. Sell described work on inertial manifolds aimed at simplifying and rendering more efficient calculations described by Derby. An inertial manifold for a particular partial differential equation is an attracting positively-invariant subset of the infinite-dimensional solution space which allows for meaningful projection of the partial differential equation to a set of M ordinary-differential equations. In essence, inertial-manifold projection aims to improve standard (e.g., finite-element, spectral) projection methods for low-dimensional systems by using information on the underlying dynamics to reduce M. Sell indicated that although the Navier-Stokes equations are not yet known to have an inertial manifold, they are known to have an approximate inertial manifold which inherits much of the dynamical significance of the "real thing". Although Sell indicated that the procedure for determining approximate inertial manifolds is known, the techniques have yet to be applied to any moderately real problems, and thus the computational complexity (and hence utility) of the procedure has yet to be determined. Discussions did not proceed far enough for meaningful examples

to be offered for other than linear parabolic systems. In essence, the talks of Derby and Sell were still too decoupled to judge the success of the concept.

S. Orszag introduced the fundamental problems associated with the calculation of turbulence in fluid flows, and presented several new approaches to the problem. Orszag described the general techniques available for turbulence prediction, including full simulation, large-eddy simulation, and transport-model approaches, and related the trade-off of complexity and precision in each. Orszag also described the symbiosis between the techniques, in that full-simulation results allow for detailed flow inspection and subsequent development of better transport models. The former were illustrated by recent numerical experiments on the structure of turbulence and nonlinear depletion, the latter by an exposition of the renormalization-group method (RNG) for generation of sub-grid-scale and transport models of turbulence. The RNG approach allows, with certain assumptions, for the direct calculation of the"constants" of turbulence and turbulence models, and provides a general framework in which to evaluate the effect of new physics. Orszag described several successes of RNG, including applications to stratified flows and high-speed compressible flows.

In addition to the invited talks, Auslander commented on several other interest areas of the ACMP, in particular on the computation aspects of the ACMP. He indicated that improvements in algorithms are a key step towards effective use of new-generation computers - a conclusion borne out in a recent ACMP/DSO-sponsored workshop at Caltech (June 19-21), in which vendors described a level playing field as regards hardware, with discrimination and market-share depending critically on software. Auslander cited specific ACMP efforts in parallel algorithm development, use of parallel architectures in

discipline-driven research (e.g., materials science), development of new signal analysis and signal processing algorithms, and the development of new algorithms for nonlinear problems. It was the consensus of the MRC members in attendance that the ACMP has the right mix of "Applied" and "Mathematics", that the work being supported is of high caliber, and that the ACMP Principal Investigators are clearly interested in "interdisciplinary" research involving both mathematics and the client sciences. The work presented very nicely combined fundamental contributions with near-term applicability.

As regards the relevance of the work to the DoD effort, it is clear that the ACMP effort is directly relevant to subjects ranging from materials science and materials processing to the design of submarines and aircraft. It was difficult to judge the full scope of the ACMP from this small sample. However, it would seem from Dr. Auslander's comments, and from the sample presented, that the challenging problems in the stressing, flow, and fracture of solids, and in the interactions of microscopic and continuum approximations, highlighted in a 1988 MRC meeting, have not yet been given serious consideration by the ACMP.

Recommendations for Future ACMP Conferences at MRC Meetings:

1. The conclusions above are drawn from the small sample size of four speakers - in future years, a two-day conference would be preferable in order to get a better sense of the ACMP program as a whole. The second day of the conference could easily overlap with an orthogonal MRC conference.

2. The MRC (or an easily defined MRC math subgroup) did not have sufficient input into this year's meeting. In the future, at least a few of the talks

should be given by MRC-invited speakers, preferably on topics not currently supported by ACMP, but of interest to DSO, DARPA, or DoD.

3. Few MRC members are familiar in much detail with some of the fields represented in the ACMP (especially notable in this regard are signal processing, control, and turbulence flow). Not being familiar with the fields, one is not aware of the key problems in the field, the competing concepts, the limitations and drawbacks of proposed methods, or the appropriate metrics by which to measure success. In future years, there should be several (e.g., two) invitees in each field (not necessarily both ACMP), preferably with somewhat different perspectives or viewpoints. This should prove useful to the Program Director, as well as provide the dialectic necessary for critical evaluation by the MRC.

4. Professor Auslander's tenure at DARPA is scheduled to end in FY '91. MRC-ACMP interactions are imperative if the MRC is to play an effective role in planning and ensuring continuity of the potentially high pay-off ACMP program.

AGENDA

MATHEMATICAL MODELING MEETING

July 13, 1989

ORGANIZER : Dr. Louis Auslander

Thursday, July 13

HERB LEVINE (U.C.S.D.) : Crystal Growth As An Example of A Free Boundary Problem

STEVE BOYD (Stanford University) : Optimizing Multi-Sensing Feedback Systems for Manufacturing Process

GEORGE SELL (University of Minnesota) : Applications of Inertial Manifolds to Problems in Chemical Engineering

STEVE ORZAG (Princeton University) : Non-Linear P.D.E. and Applications

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DESIGNING WITH ADVANCED COMPOSITES

A. G. Evans, B. Budiansky, J. W. Hutchinson, J. C. Williams, B. Wilcox, W. Barker

EXECUTIVE SUMMARY

A meeting held in accordance with the attached agenda provided a designer perspective on research needs required for the development of design codes applicable to advanced structural materials. The design group recognize that existing codes for alloys are not applicable. Successful utilization of these materials requires new design codes, developed through close collaboration between materials and design engineers. To facilitate the process, much can be gained from design practice already developed for polymer matrix composites. These procedures accept that low ductility is given and furthermore, successful utilization of advanced materials accepts the incidence of controlled structural separations.

Design codes for advanced composites must be flexible to accommodate different matrix properties and hence, different prevalent failure modes. In particular, acceptable ductile matrix composites (metal and thermoplastic matrices) have sufficient transverse mechanical properties that structural integrity in engine applications appears to be limited by thermal/mechanical fatigue. However, present fatigue-based design codes used for alloys are not applicable to composites. New design approaches must be devised, facilitated by model-based criteria for fatigue crack growth and residual strength, coupled to features of the matrix damage amenable to non-destructive characterization.

Adequate brittle matrix composites invariably have low shear and transverse tensile properties. Laminated and/or woven architectures are thus required, whereupon delamination is a prevalent failure mode. Test procedures

and models that establish mixed mode delamination criteria are a priority for design codes applicable to these materials. Some of these already exist for polymer composites, but need to be adapted to intermetallic, ceramic and carbon matrix systems. Experience with polymer systems suggests that stitched fiber effects should be an integral aspect of delamination criteria.

Damage tolerance can be built into composites by the judicious use of buffer layers that control damage propagation. This approach has been successfully utilized for polymer systems. However, criteria that prescribe the mechanical properties and geometric characteristics of buffer layers must be devised for their effective utilization.

Attachments and diffusion bonds between composite and monolithic components and section changes in composite components are areas of concern. Fiber terminations in these areas result in strain concentrations which can exacerbate fatigue and delamination. Research that provides knowledge of material behavior in these regions is regarded as a priority.

INTRODUCTION

A spectrum of high performance fiber reinforced composites is now in an advanced stage of development. However, there is limited experience in designing components with these materials. Indeed, the apparent mechanical properties of advanced composites fall outside the range encompassed by conventional design codes. It has thus become clear that a design/material dialogue is essential to the successful utilization of these materials. The intent of the meeting was to initiate such a dialogue.

A prevalent feature of fiber reinforced materials is low conventional "ductility" (rupture strains of ~1 percent) and the incidence of damage prior to

rupture. Both of these features are regarded as unacceptable in conventional design practice. However, these materials can have high specific strength and excellent damage tolerance: properties of substantial importance in high performance structures. A design process is required that utilizes these advantageous properties, while diminishing the detrimental structural impact of damage and low ductility. Much experience with these issues has been gained with polymer matrix composites, but the process has only just begun with metal matrix, ceramic matrix and carbon/ carbon composites. Such experience has indicated that the effective utilization of composites involves loadings that inevitably cause stable damage. A design approach that accepts the presence of damage and its effect on structural performance is thus required.

PROPERTY CHARACTERISTICS

Some common mechanical features of fiber reinforced materials are summarized in Table I. Subject to axial loading and in the absence of notches, ultimate failure is essentially mode I, (i.e., a "fracture plane" normal to the stress axis). However, in all cases, damage occurs in the form of either matrix cracks or fiber cracks. Furthermore, except in ductile metal matrix systems, the damage can only be stabilized (i.e., non-catastrophic) by introducing a fiber/matrix interfacial zone subject to debonding and sliding (Fig. 1). The latter represents another mode of damage, now at interfaces, which must be present in ceramic, intermetallic, carbon and polymer matrix composites. Additionally, as elaborated below, interface damage appears to be an important aspect of fatigue resistance in metal matrix composites.

TABLE I

SOME COMMON MECHANICAL CHARACTERISTICS OF ADVANCED COMPOSITES

PROPERTY	MECHANISMS
DUCTILITY	LIMITED BY FIBER BUNDLE STRAIN
TENSILE STRENGTH	INHERENTLY ANISOTROPIC AXIAL <--> FIBERS: TRANSVERSE <--> MATRIX
TOUGHNESS (NOTCH SENSITIVITY)	LARGE "MODE I " RESISTANCE (CHARPY) MIXED MODE DELAMINATION
SHEAR STRENGTH	MATRIX DAMAGE COALESCENCE
DAMAGE	MATRIX CRACKS FIBER CRACKS INTERFACE DEBONDS

In the presence of notches, other failure modes can occur. Most significantly, mixed mode delamination is present (Fig. 2) in brittle matrix composite such as ceramic, carbon and resin matrix systems and can also exist in intermetallic and metal matrix systems with appropriately designed interfaces. Furthermore, delamination can occur during fatigue in notched metal matrix composites. Delamination ameliorates notch sensitivity and results in enhanced (sometimes substantially) Charpy energy. However, the transverse and shear strengths of the composite diminish as delamination is enhanced. Design analyses are needed to understand acceptable compromises in the property set which occurs when delamination is involved.

The transverse tensile strength is particularly low in brittle matrix composites because interface debonding is a prerequisite for acceptable axial properties. This strength is largely governed by the matrix fracture toughness and also tends to diminish as the fiber diameter increases. Consequently, ceramic, carbon and polymer matrix systems are typically more anisotropic than metal and intermetallic systems. Either laminated or woven structures are always needed whereupon multiple cracking of the matrix and/or the interfaces is inevitable and must be included in design concepts. Additionally, the materials must be able to withstand the presence of damage in the environments of practical relevance, with attendant implications for the choice of fiber and of fiber coating.

Rapid progress has occurred in understanding the incidence and extent of damage in composites and this progress will continue for the next several years within the framework of the URI Composites programs. The challenge for the materials/mechanics/design community thus appears to involve the translation of the micromechanics formulations of damage into simple constitutive laws that can be used for design calculations. Furthermore, design calculations based on these laws will provide a much needed focus on a property set suitable for further materials development.

DESIGN

Design requirements for composites are not accepted to be universal because the damage modes and the anisotropies depend upon the ductility/toughness of the matrix. It is probably appropriate to discuss separately ductile matrix systems and brittle matrix systems. However, several common features can be first addressed.

Ductility does not appear as a specific parameter in design codes and is seemingly an unimportant consideration in performance. However, experience has indicated that some ductility is needed to prevent damage during handling and assembly. Requisite levels of ductility are thus qualitative and experience-based. For present purposes, it is simply noted that alloys having ductilities of order 2 percent are now in use in engines and that polymer composites being used have ductilities of ~0.5-1 percent. The toughness and/or Charpy energy are also only implicit parameters in design. However, residual life after fatigue is governed by toughness and is an important aspect of the present ENSIP approach. Additionally, low cycle fatigue life is associated with stress concentrations and is related to toughness. Specific use of toughness in advanced design codes could thus be envisaged.

It is now accepted that new design approaches are needed for composites (through close cooperation between materials and design engineers) and furthermore, that design rules must be sufficiently flexible to accommodate differing behaviors between these various classes of composite.

Ductile Matrix Composites

Metal matrix composites (MMC) processed to avoid both appreciable fiber degradation and reaction products which embrittle the matrix have good axial and transverse tensile properties. The resultant high specific strength and modulus are very attractive features of these materials, suggesting several potential applications in high thrust to weight engines (Fig. 3), etc. Present understanding of these materials indicates that performance in engines is limited by mechanical/thermal fatigue. These processes involve matrix cracking with matrix crack nucleation occurring readily at either cracked fibers or from

reaction product layers. Fatigue performance thus appears to be propagation dominated. Consequently, present design practice for engines, which requires that initiation life meet the design life must be abandoned. Instead, rigorous understanding is needed of fatigue crack growth and relations developed between crack growth and residual life through appropriate NDE. A near term focus on this issue is regarded as extremely important. It is believed that this process will be facilitated by development of a micromechanical model (analogous to matrix cracking in brittle matrix composites) which identifies the role of the fiber and the fiber/matrix interface, as exemplified in Appendix I. Such analysis will help parameterize history effects and residual life.

Thermal fatigue and coupled thermal/mechanical fatigue are also prevalent in composites. The former is often dominated by the misfit strain, e_t, that originates with the mismatch in thermal expansion between the fiber and matrix. Limited experience indicates that matrix fatigue failure occurs rapidly when $e_t>e_o$ (the matrix yield strain) because of reversed plasticity in the matrix upon thermal cycling. However, when $e_t>e_o$, shakedown is followed by essentially indefinite lifetime. The known incidence of rapid thermal fatigue provides bounds on the acceptable choice of fibers for each matrix system. For example, it appears that SiC fibers are not applicable for TiAl matrices. However, based on acceptable fiber choices, it will be necessary to investigate coupled thermal/mechanical fatigue below the thermal fatigue limit, suitable for use in design analysis.

In addition to fatigue, the basic principles involved in joining and/or attachments are yet to be developed. Diffusion bonding is presumed to be the preferred approach with the composite bonded, say, to the matrix alloy. Failure modes in this region, such as fatigue, caused by the property mismatch are

apparently unknown and need to be investigated at a level suitable for design. A related problem occurs at section changes where fibers are discontinued, leading to local strain concentrations.

Ductile thermoplastic matrix (e.g, PEEK) composites exhibit many of the above fatigue limited structural characteristics. Emerging experience with these composites should facilitate the development of design concepts for metal composites.

Brittle Matrix Composites

Design with brittle matrix composites has a basis in polymer matrix systems (Fig. 4) which emphasizes concurrent engineering and a broad experience base in the conceptual design phase. Cautious extension of the approach to other composites may be completed.

A prevalent mode of structural failure in brittle matrix composites is delamination, which can occur in accordance with the range of mode mixities (shear/tension) (Fig. 5), subject to either mechanical or thermal loads and complicated by anisotropy. Test procedures that characterize the delamination resistance over the range of have been developed and provide design input. When the calculated in-plane shear and transverse tensile stresses exceed the critical delamination conditions, experience has indicated that the optimum approach is to redesign until a design is produced that avoids delamination. When this is not possible, stitching to introduce fibers normal to the predicted delamination plane can be used to inhibit this mode of failure. Experience indicates that about 10 volume percent of fibers provides adequate delamination resistance when a good design is used.

While it is essential to recognize that delamination is a key failure mode in these materials and while preliminary design notions regarding its avoidance exist, a research activity that provides a rigorous understanding of this phenomenon would be an important input to design codes. Some preliminary research has been done using modern concepts of mixed mode fracture at interfaces in anisotropic media, developed in the URI programs. An emphasis on further research of this type is a priority for the URI and related programs, including the influence of stitched fibers normal to the crack plane.

The attributes of the pseudo-ductility that exists in these materials, beyond the ultimate stress (Fig. 6), caused by matrix cracking and fiber pull-out, have been subject to initial design investigation. In particular, the effect of this material damage on the alleviation of the stress around holes within thin plates has been estimated using a damage formulation based on Weibull statistics and fiber pull-out. The implications can be addressed within the context of primary, unconstrained (P) stresses and secondary, constrained (Q) stresses. The former is exemplified by a large hole in a narrow plate: a configuration for which the allowable maximum stress intensity is less than the maximum stress in the uniaxial stress/strain curve. The latter is reflected in the behavior of a small hole in a wide plate. In this case, the allowable maximum stress range should be less than twice the maximum stress in the uniaxial stress/stress curve. Finally, for displacement controlled cases, such as thermal strains, "the ductility" is even more beneficial in assuring structural integrity.

A final point concerns the use of buffer layers within the composite structure, (Fig. 7). These are layers having low modulus and appreciable ductility, well bonded to the composite, e.g., matrix-only layers. These layers when judiciously designed into the structure, can arrest and blunt crack-

damage in the composite layers leading to substantially improved structural integrity. This concept is presently qualitative, but has been used with considerable success in polymer matrix systems. A rigorous description of the damage arrest process would allow buffer concepts to be routinely incorporated into design codes.

SUMMARY AND RECOMMENDATIONS

It is now (finally) recognized that the successful utilization of advanced structural materials requires new design codes: existing codes for alloys are inappropriate. Furthermore, it is appreciated that the timely development of such codes requires a close collaboration between material and design engineers. A format that encourages this collaboration should be implemented soon.

A design process exists for polymer matrix composites. Much of this can and should be translated to design codes used for other advanced materials. This design process accepts that controlled structural separations are inevitable if the materials are to be successfully utilized and, furthermore, that structural components having ductilities in the range 0.5 to 1 percent can, indeed, satisfy requirements of structural integrity. A program that provides for the broad acquisition of this design knowledge by the MMC, CMC and C/C design groups should be initiated.

Design for ductile and brittle matrix composites requires different emphasis and design codes must have sufficient flexibility to accommodate different matrix properties.

Ductile matrix composites, such as Ti alloy systems, have sufficient transverse strength that the limiting structural property is fatigue: both

mechanical and thermal. An additional consequence of the good transverse strength is that uniaxial reinforcement is often practicable. Present design procedures for fatigue are not applicable to composites. New design procedures that emphasize crack growth (da/dn) rules and relevant non-destructive damage evaluation must be devised. This process will be facilitated by a URI Research emphasis on a model-based understanding of fatigue crack growth and residual strength in fiber reinforced alloys. Such a study should attempt to relate fatigue damage to residual life.

Brittle matrix composites having satisfactory axial properties inevitably have relatively low transverse/ shear strengths. Consequently, structural components require either laminated or woven architectures. A consequence is the incidence of mixed mode delamination as a prevalent failure mode. Design codes thus require delamination criteria based on the magnitudes of the in-plane shear and transverse tensile stresses. The development of test procedures and models that establish these criteria should be an important emphasis of URI programs on these materials. Some of these exist in the polymer composites field and should be adapted to other systems. A feature of this activity should be an understanding of the effect of a small volume fraction of stitched fibers on the delamination criteria.

Buffer layer concepts for the enhancement of structural integrity, successfully utilized for polymer systems, have important implications. Model based criteria for the properties and geometric requirements applicable to these layer are needed for implementation in design codes.

Attachments and diffusion bonds between composite and monolithic components and section changes in which fibers terminate are areas of concern. These areas are subject to delamination in brittle matrix composites

and are presumed to be susceptible to fatigue in ductile matrix composites. Criteria for designing these regions do not exist. Initiation of research is this area is of paramount importance.

APPENDIX I

MATRIX FATIGUE CRACKING IN FIBER COMPOSITES

Various regimes of fatigue crack propagation seemingly exist in fiber reinforced-metals. One regime is analogous to matrix cracking in brittle matrix composites, wherein the fibers remain intact as the crack extends through the matrix. This behavior is made possible by having a interface that debonds and slides in preference to fiber cracking. Such behavior is characteristic of SCS6 fibers which debond and slide along the C coating layer and have high tensile strength.

The characteristics of fatigue crack growth in the composite may be evaluated by determining the bridging effect of intact fibers and by allowing matrix crack growth to occur in accordance with a conventional Paris law

$$da/dN = A\Delta K_{tip}^{n} \qquad (1)$$

where K_{tip}^{n} refers to the matrix crack front.

Using the formalism for matrix cracking, McMeeking has shown that, in steady-state,

$$\Delta K_{tip} = \sqrt{\frac{2}{3}} \left[\frac{(1-f)\,R\,E_m{}^2}{8\,(1-v^2)f^2E_fE\tau}\right]^{1/2} (\Delta\sigma)^{3/2} \qquad (2)$$

where τ is the interface sliding stress, E is Young's Modulus and $\Delta\sigma$ is the stress range. By combining Eqns. (1) and (2) it is evident that da/dN depends on

$\Delta\sigma^{3n/2}$ and not on ΔK. There are also strong effects of τ (about 200 MPa for SCS6 in Ti alloys). For shorter cracks, when,

$$a/R \gtrsim \Delta\sigma/\tau \tag{3}$$

steady state does not apply, whereupon the crack growth rate is governed by:

$$\Delta K_{tip} \leq \Delta\sigma\sqrt{\pi a}\left[\sqrt{1+\frac{B^2\tau a}{R\Delta\sigma}} - B\left(\frac{\tau a}{R\Delta\sigma}\right)^{1/2}\right]^2$$

where

$$B^2 = \frac{2.33f^2 E_f E (1-v^2)}{(1-f)E_m^2}$$

Some typical trends are sketched on Fig. A1.

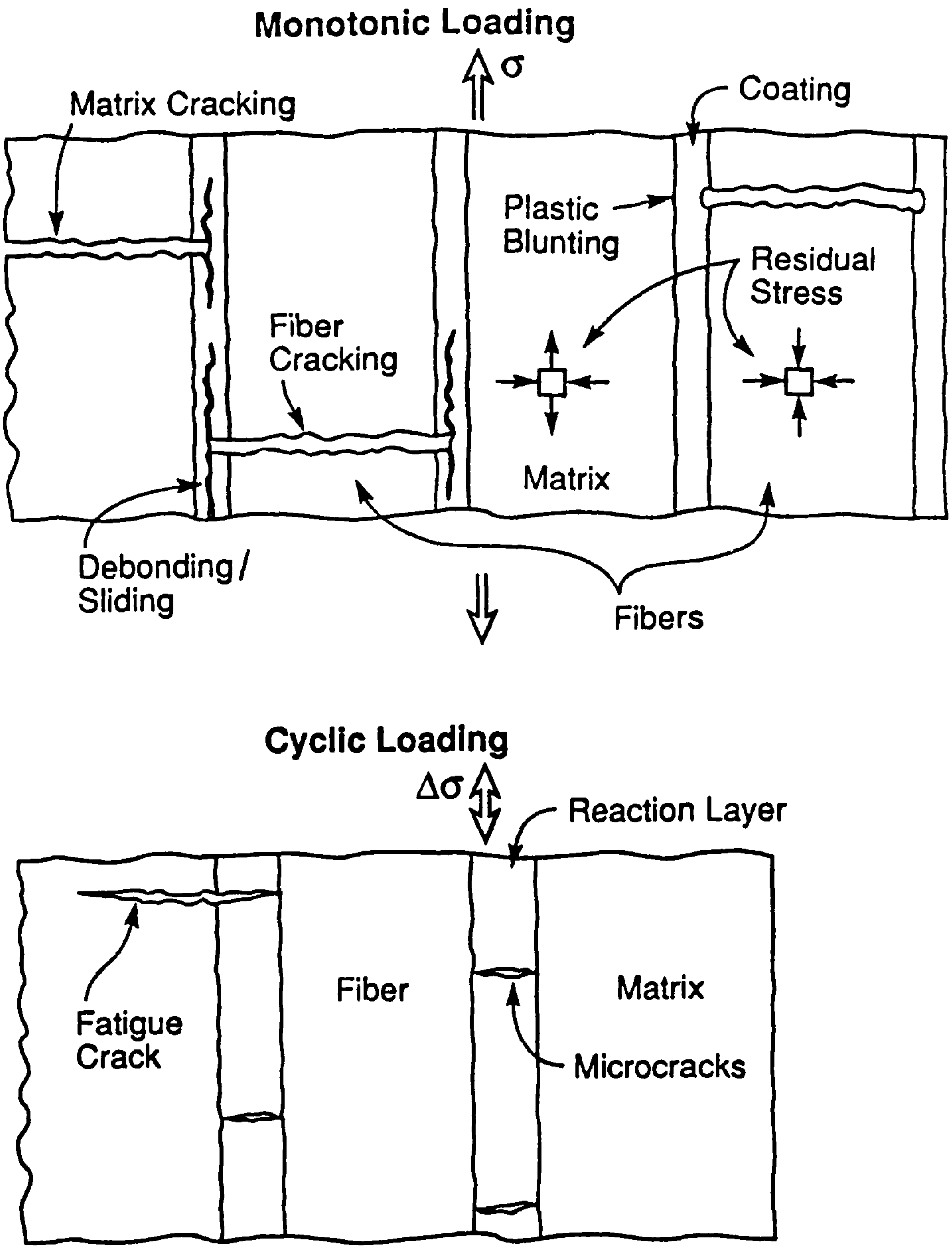


Figure 1. The response of the interface in composites to cracks occurring in the fiber and in the matrix.

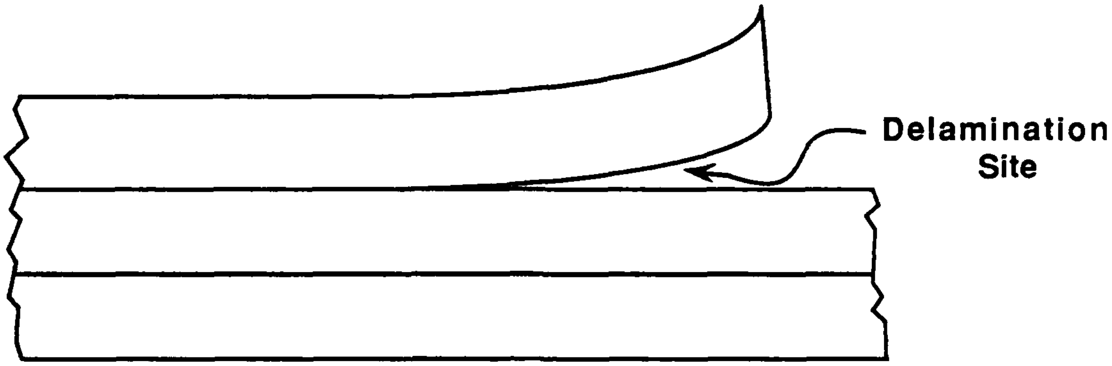


Figure 2. A schematic of delamination cracking in composites.

Potential Applications for Titanium Alloys/MMC's

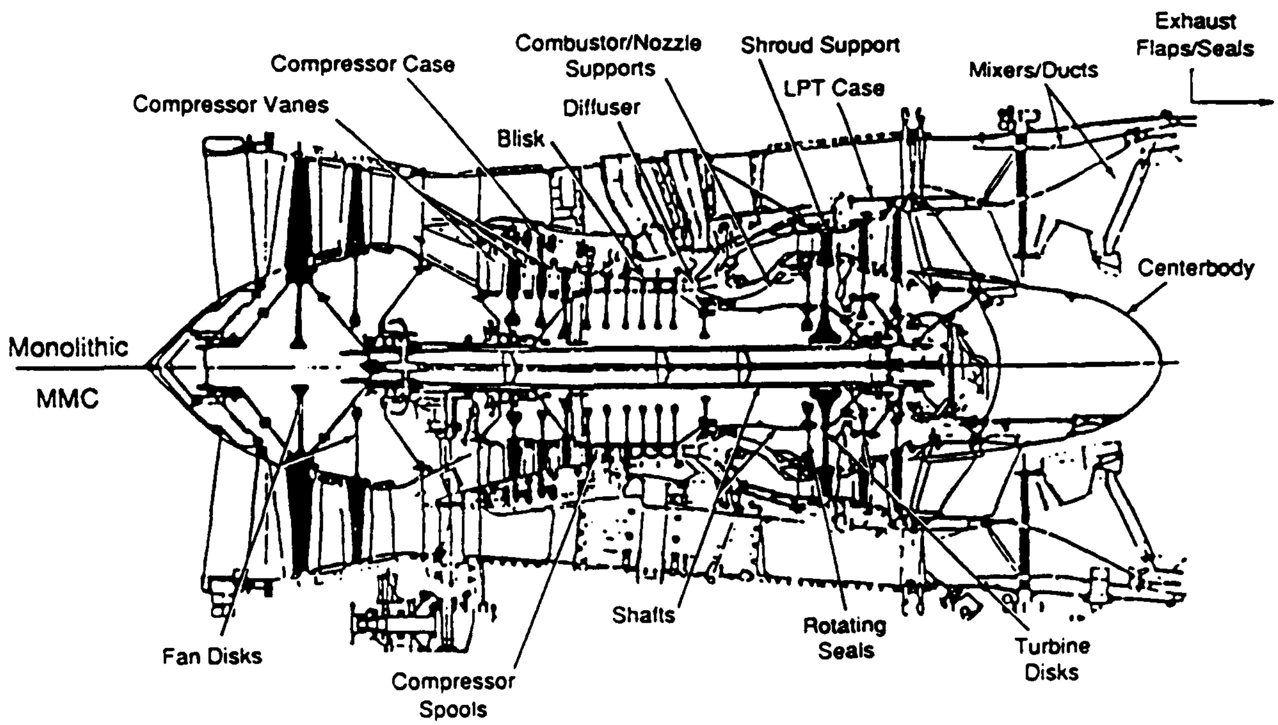


Figure 3. Areas within an engine amenable to MMC.

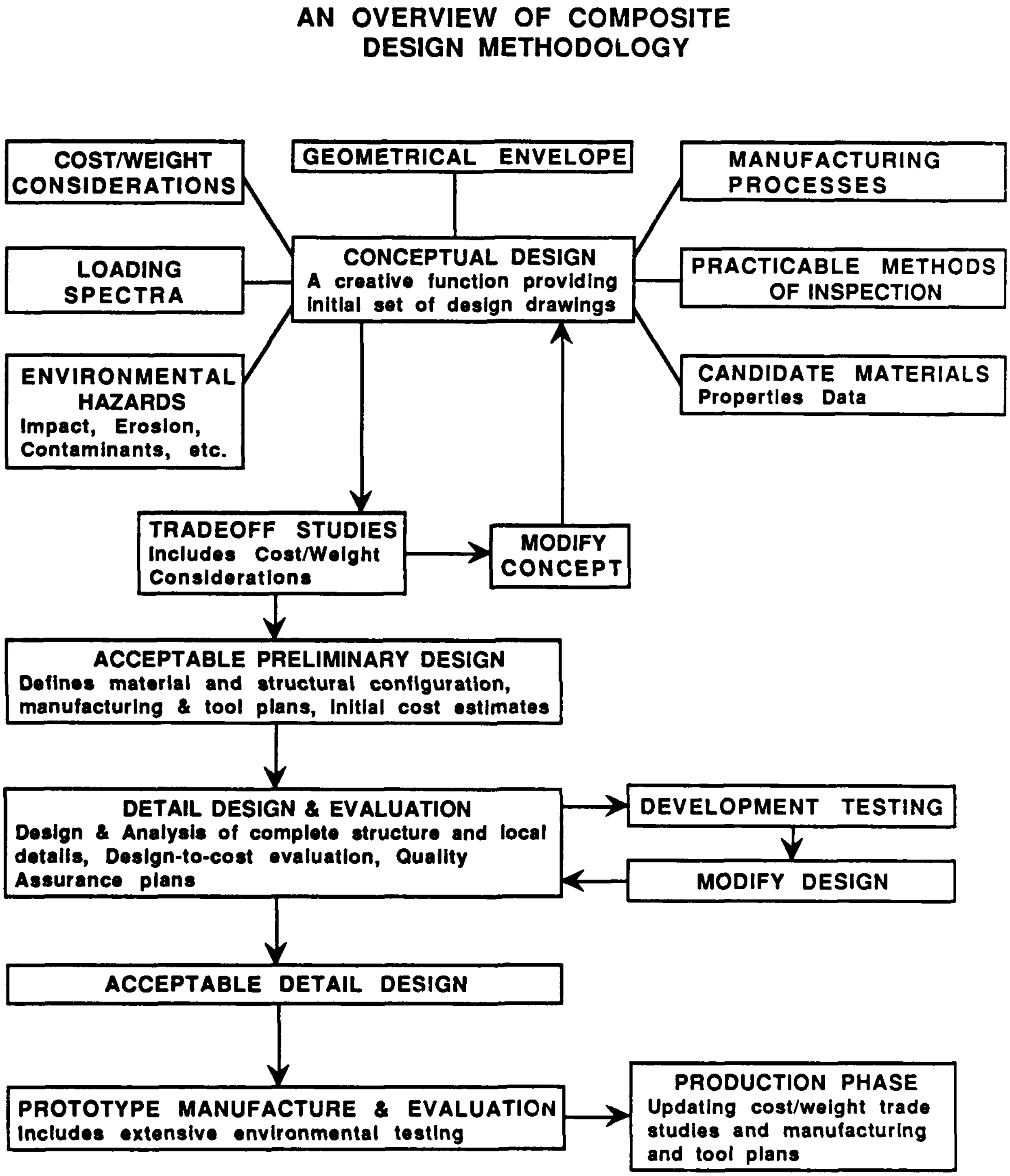


Figure 4. A design process for Advanced Composites.

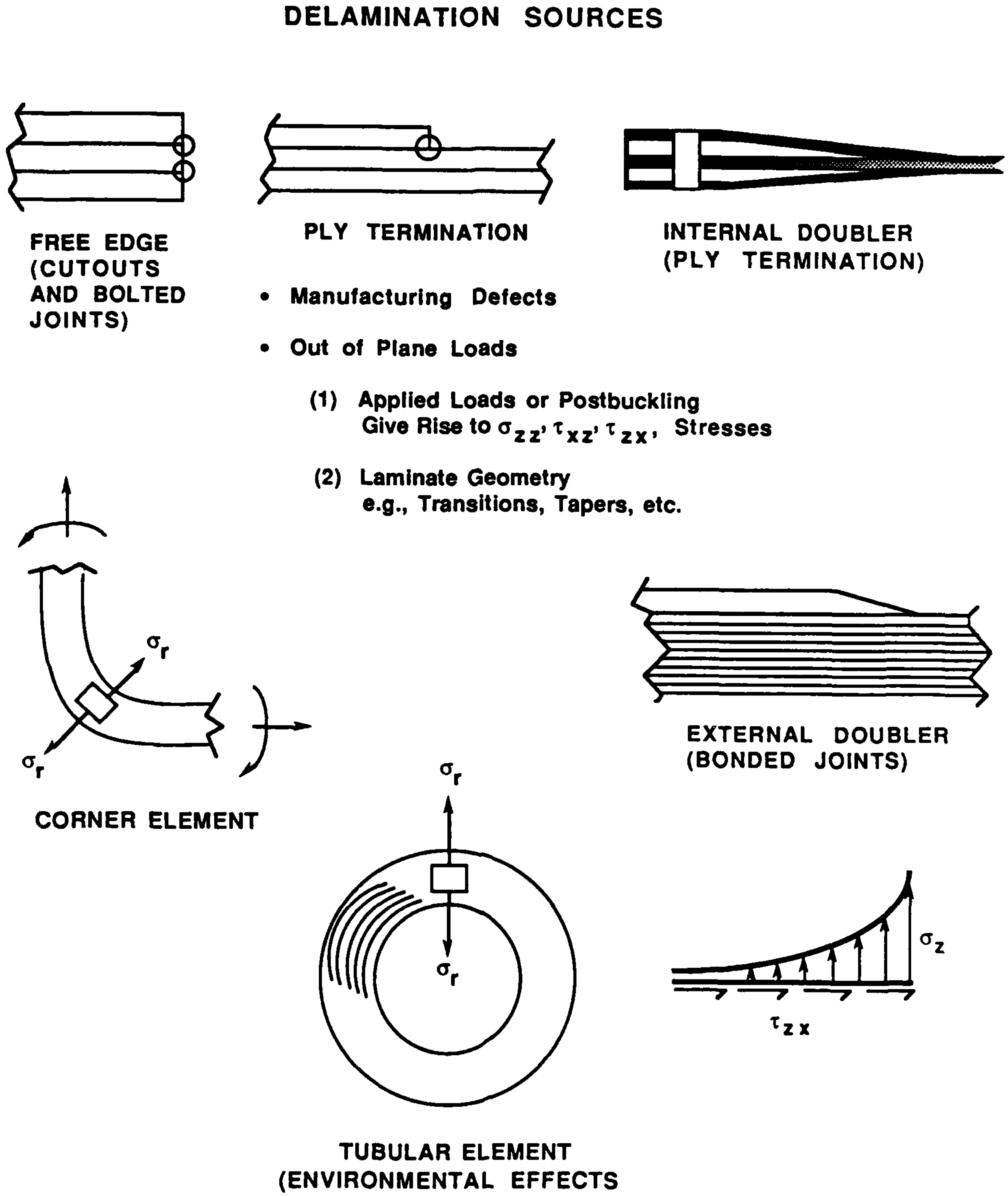
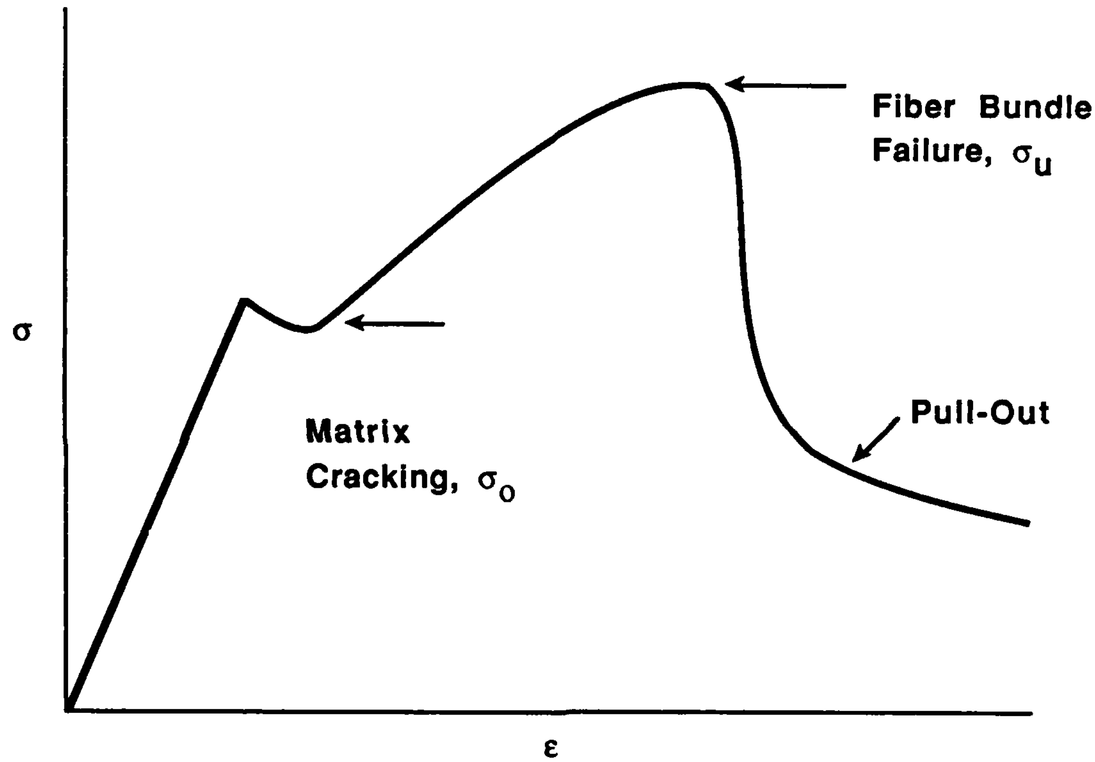


Figure 5. Sources of Delamination in Composites.



a) 'Tough' Composite

Figure 6. Pseudo-ductility in brittle matrix composites.

CRACK ARRESTMENT OF "BUFFER" STRIP CONCEPTS CAN IMPROVE FRACTURE TOUGHNESS OF LAMINATES IN THE AREA OF BOLTED JOINTS

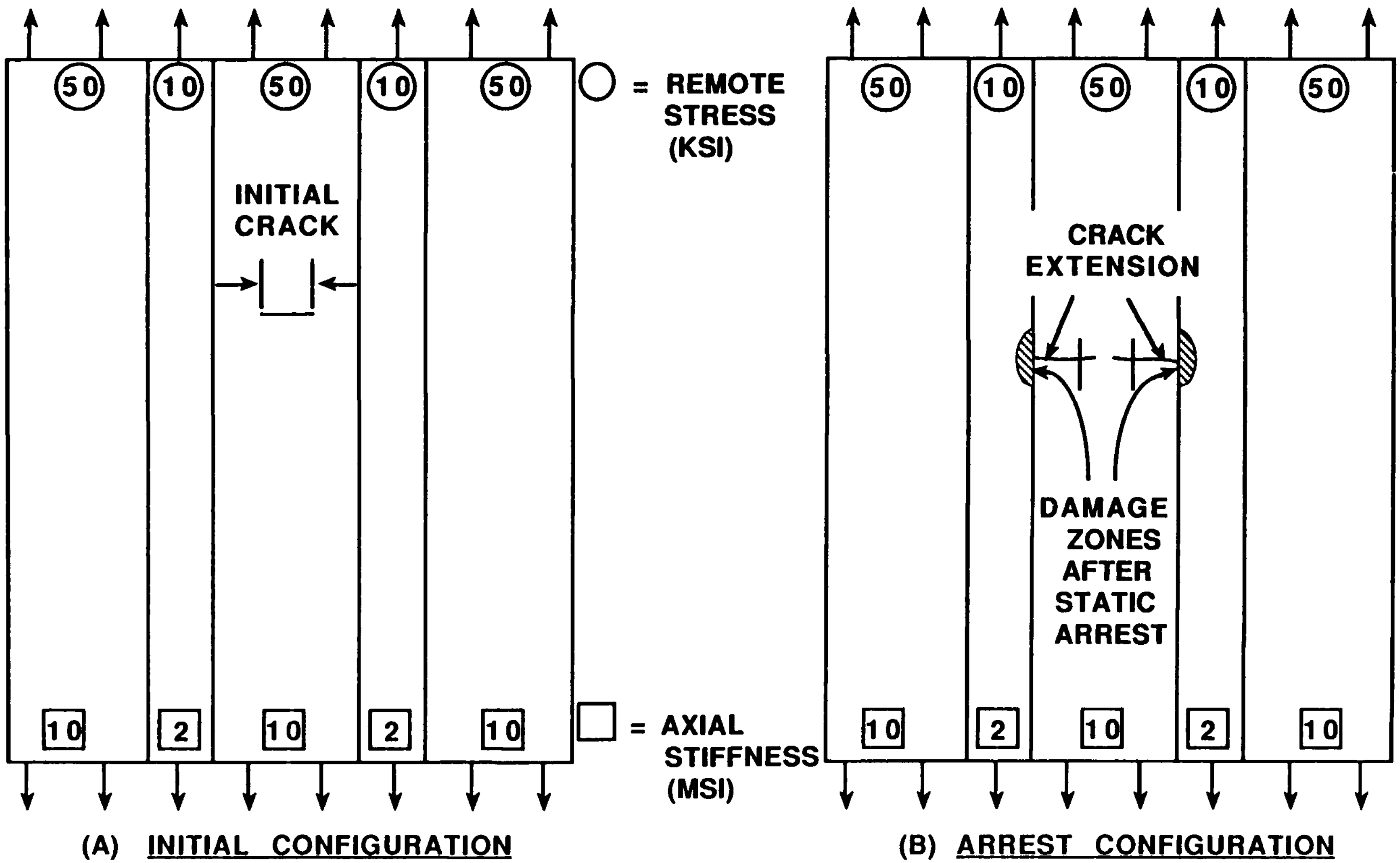


Figure 7. The buffer layer concept for structural integrity.

AGENDA

DESIGN PRINCIPLES FOR AGVANCED STRUCTURAL MATERIALS

July 14, 1989

OBJECTIVES:

Traditional alloy systems have requirements for ductility, high toughness, etc. Many of the newer, light weight materials such as intermetallics, ceramics and composites have essentially zero ductility and only moderate toughness. The design of components using these materials thus requires a modified design philosophy. The objective of this meeting is to discuss a design approach for these materials consistent with "zero" ductility, property anisotropy and damage. The meeting begins with presentations concerning the known properties of these materials, followed by experiences thus far in design. The afternoon will then be devoted to such questions as: What "toughness" is needed; can damage, such as matrix cracking, be tolerated, etc.

Friday, July 14

Mechanical Characteristics of Advanced Composites - A. G. Evans,
B. Budiansky (MRC)

Design Experience With Advanced Engines - M. VanWanderham, Pratt & Whitney

Designer View of Titanium Aluminides and MMC's - C. Haubert, G. E. Aircraft

Design Procedures for Composites - K. Kedward, McDonald Douglas

Airforce Propulsion Lab Perspective on Titanium, Aluminides and MMC's -
T. Fecke, Airforce Propulsion Lab.

Constitutive Laws For Advanced Composites - F. A. Leckie, UCSB and
D. Hayhurst, Sheffield University

Discussion: The roles of ductility, toughness and damage in the design of components using advanced composites.

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THE FRACTURE ENERGY OF METAL/CERAMIC INTERFACES

B. Budiansky, A. G. Evans, J. P. Hirth, J. W. Hutchinson, J. R. Rice

A number of metal/ceramic interfaces exhibit brittle fracture, but with fracture energies Γ_i substantially in excess of the work of adhesion, W_{ad}. One example is the Au/Al_2O_3 interface for which $\Gamma_i \approx 50 Jm^{-2}$ and $W_{ad} \approx 0.5 Jm^{-2}$. The substantial magnitude of $\Gamma_i/W_{ad} \approx 10^2$ has been attributed to plastic dissipation occurring in the Au layer. Yet, there is a fundamental paradox in the analysis that attempts to relate the plastic dissipation to the variables in the problem. Notably, the maximum stresses attained from continuum analysis, near the crack tip, are ~3-5σ_0, where σ_0 is the uniaxial yield strength. Yet, brittle fracture by bond rupture at the crack tip is stress controlled and requires stresses or order $\mu/20$, where μ is the shear modulus (in accordance with the stress/displacement law depicted in Fig. 1, and subject to the energy, $W_{ad} \approx \mu b/20$, where b is the Burgers Vector). This paradox has lead to unresolved debates about connections between Γ_i and W_{ad} and, in particular, to whether the fracture energy can be formulated multiplicatively with W_{ad},

$$\Gamma_i = XW_{ad} \tag{1}$$

where X is a parameter governed by the plastic dissipation. A related issue concerns the set of observations on debonding of hard particles during tensile testing of metals which suggest that the plastic strain level is an important parameter in the debond process and not just the stress.

An attempt to reconcile the paradox recognizes a duality of plastic flow. At the continuum level plastic flow relaxes elastic stresses. However, at a scale below

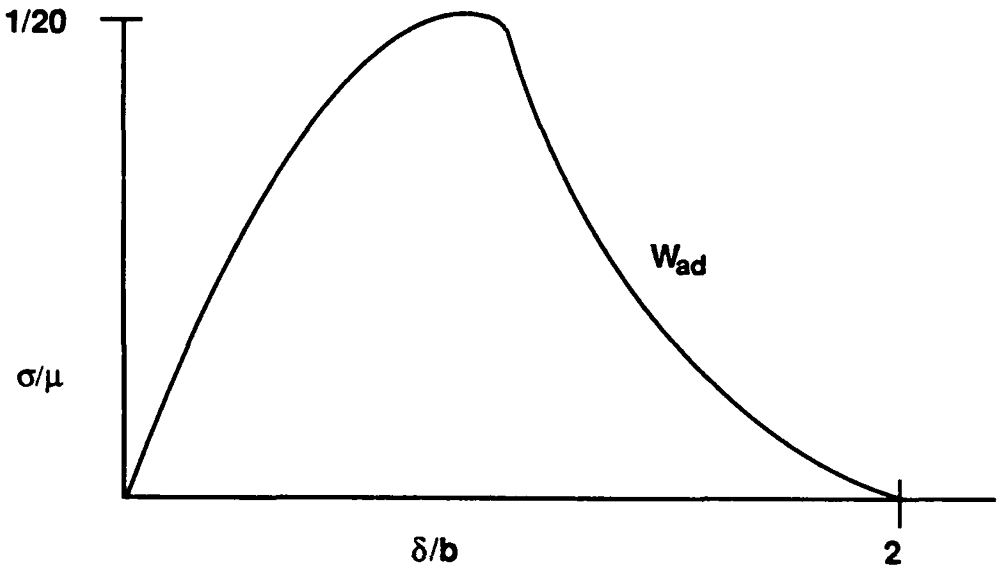


Figure 1.

the dislocation cell size, dislocation configurations (such as pile-ups) can cause large local stresses. Dislocation configurations that locally enhance the tensile stresses in the bond rupture zone may thus provide the requisite connection between the bond rupture stresses and the continuum stresses (Fig. 2).

This duality may also be conceived using an energetic argument. Those dislocations near the interface in a layer of approximate thickness,

$$\lambda \approx b\mu/\sigma_0 \tag{2}$$

will be eliminated from the crack surface by image forces as the crack extends along the interface. The stored energy per unit area associated with this dislocated layer is

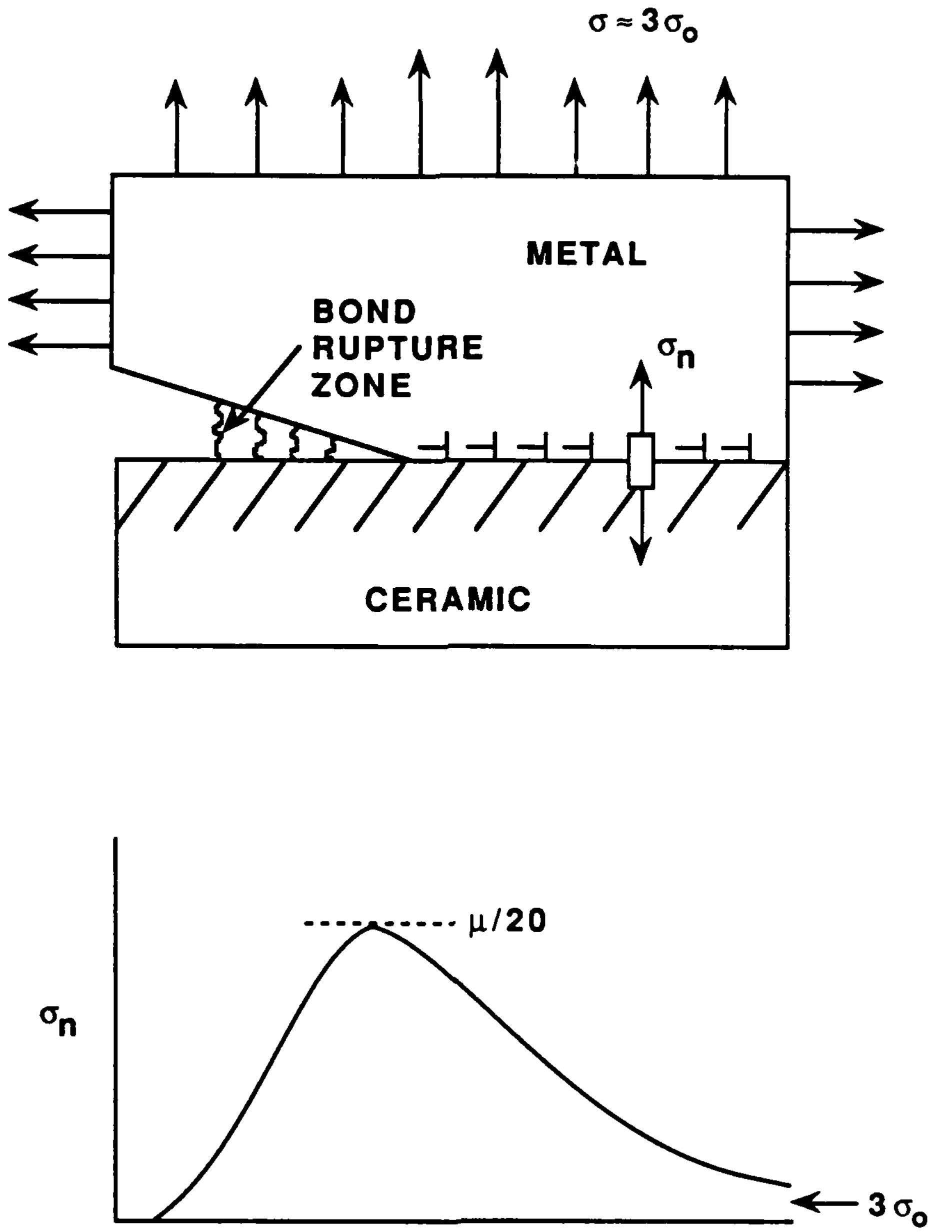
$$U_s \approx \frac{\lambda}{20}\sigma_o\varepsilon_p \approx \frac{\mu b}{20}\varepsilon_p \tag{3}$$

where ε_p is the plastic strain. The loss of stored energy may be considered as a reduction in the total energy needed to cause fracture in the bond rupture zone to

$$W = W_{ad} - U_s \tag{4}$$

That U_s and W_{ad} are about equal for plastic strains of order unity affirms the role of local dislocation arrangements on the brittle fracture process. An important influence of plastic strain on the fracture condition also emerges.

To connect the above energy based arrangement to the fracture process, specific dislocation mechanisms must be invoked. Such analysis has not been performed, but the following arguments and analogies may be noted. In brittle materials such as MgO and NaCl, dislocations have been shown to move into the region ahead of crack and enhance fracture (i.e., reduce the fracture energy), indicative of dislocations having the sign shown in Fig. 2. Furthermore, dislocations with this sign are consistent with the sign of the shear stress in the crack tip field. Consequently, a calculation may be envisaged wherein a wall of dislocations is placed along the interface, spaced according to the plastic strain just outside this zone and the requisite distribution of normal stress between $\sim 3\sigma_o$ and $\mu/20$ constructed.



STRESSES ON INTERFACE IN BOND RUPTURE ZONE

Figure 2.

TWIN INDUCED TOUGHENING IN γ–TiAl

B. Budiansky, A. G. Evans, and J. W. Hutchinson

INTRODUCTION

γ–TiAl typically has a toughness of 6-8 MPa$\sqrt{m}$. However, recent measurements performed on an alloy having composition Ti-50.5 atomic %Al homogenized at 1000°C for 20 hours have revealed a toughness of 16 MPa$\sqrt{m}$ [1]. This alloy is predominantly γ with some (<5%) α_2. One important difference between these materials is the incidence of abundant irreversible mechanical twinning that occurs in the latter upon crack growth (Fig. 1). It may be hypothesized that this twinning is the source of the enhanced toughness. This possibility is briefly explored in this note.

EXPERIMENTAL INFORMATION

γ–TiAl has a tetragonal lattice with a c/a ratio of 1.02. However, the lattice (and its defects) have characteristics typical of a face centered cubic (fcc) structure. The crystallography of twinning on {111} <112> in fcc structures is relatively well known [2], and indeed the twinning systems in γ–TiAl are of this type [3]. For these twins, the twinning <u>shear strain</u> is $\gamma_t^o = 0.707$ [2]. Measured shear strains of this order are associated with {111} <112> twins in γ–TiAl. The shear stress τ_c required to form twins may be estimated from a uniaxial stress/strain curve for this material (Fig. 2a), as being between 50 and 80 MPa.

Observations of the twins in the twin process zone (Fig. 1), indicate that the twin spacing is essentially independent of the distance from the crack plane, such that the spacing is about 100t, where t is the twin thickness. The twinning strain thus appears to saturate at $\gamma_t \approx 0.01\gamma_t^o$. This saturation behavior is

Figure 1a.

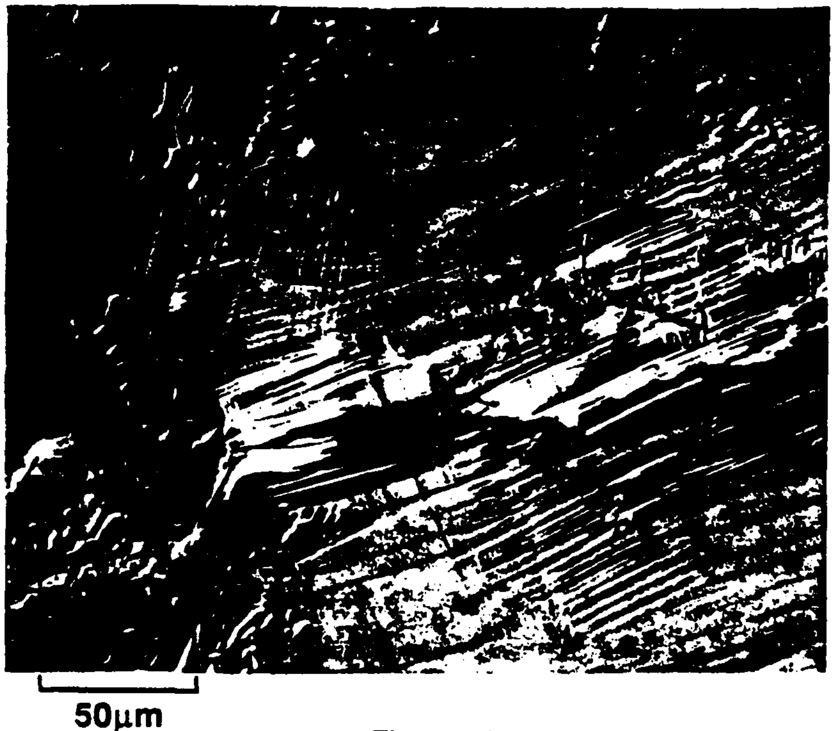


Figure 1b.

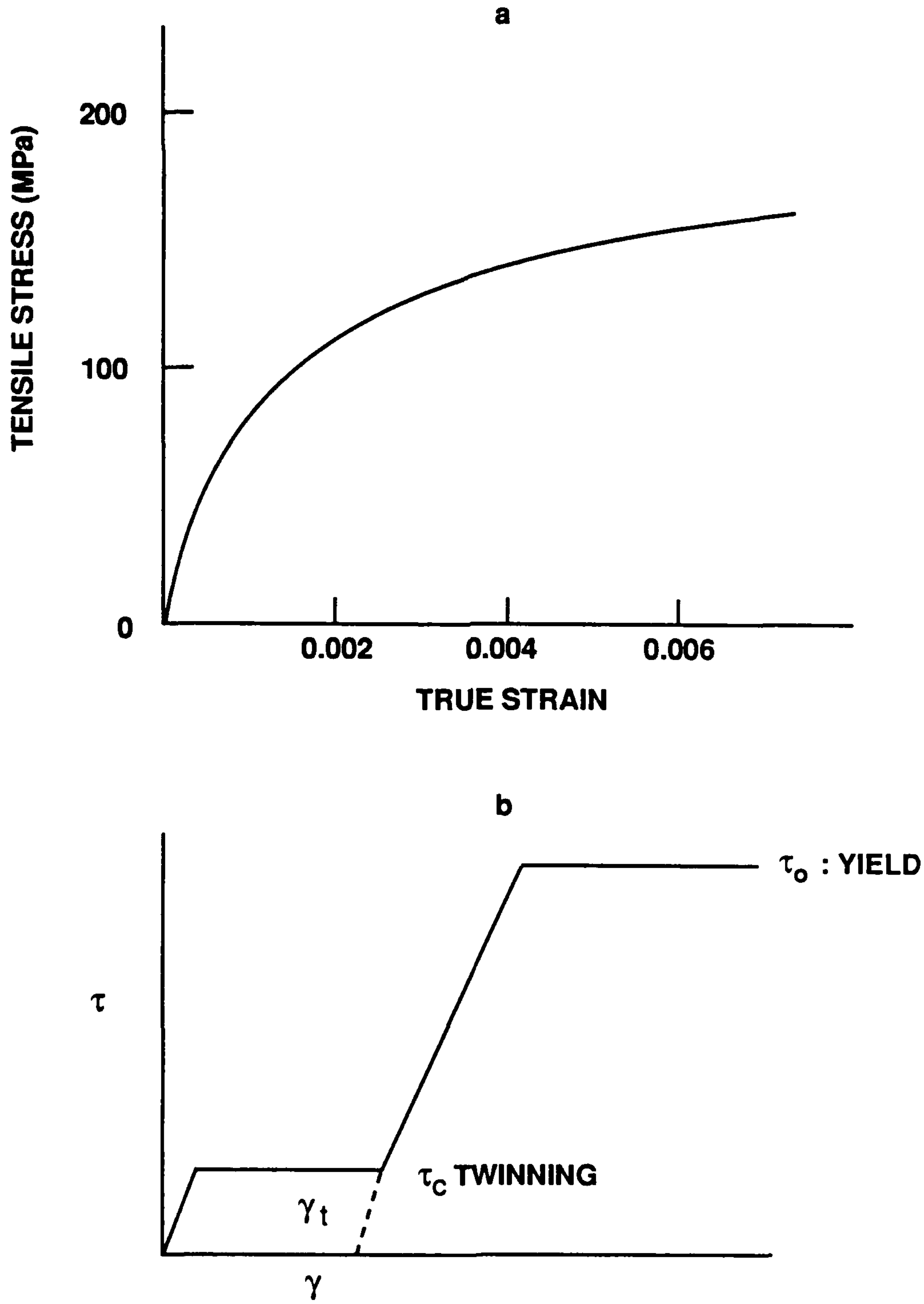

a
TENSILE STRESS (MPa)
200
100
0
0.002
0.004
0.006
TRUE STRAIN
b
τ_o : YIELD
τ
τ_c TWINNING
γ_t
γ

Figure 2.

analogous to that in the martensite transformation problem, in the sense that it leads to crack shielding with a definite stress intensity factor at the crack tip, K_{tip}. Such behavior differs, however, from normal plasticity which has no saturation strain and zero K at the tip of a growing crack. The applicability of the saturation strain concept to twinning is critical to the following derivation.

ANALYSIS

We assume that twinning planes are continuously available; that twinning will occur when the maximum shear stress τ_{max} reaches a critical value τ_c; that the full twinning strain γ_t^0, oriented in the axes of τ_{max} is induced in discrete twin bands; and that the volume fraction of twin bands is c. Thus, the effective induced twinning shear strain is $\gamma_t = c\gamma_t^0$.

During steady-state growth of a long crack (see Fig. 3) there will be symmetrical zones of twinning A, A′ above and below the crack, with leading boundaries C, C′ as shown.

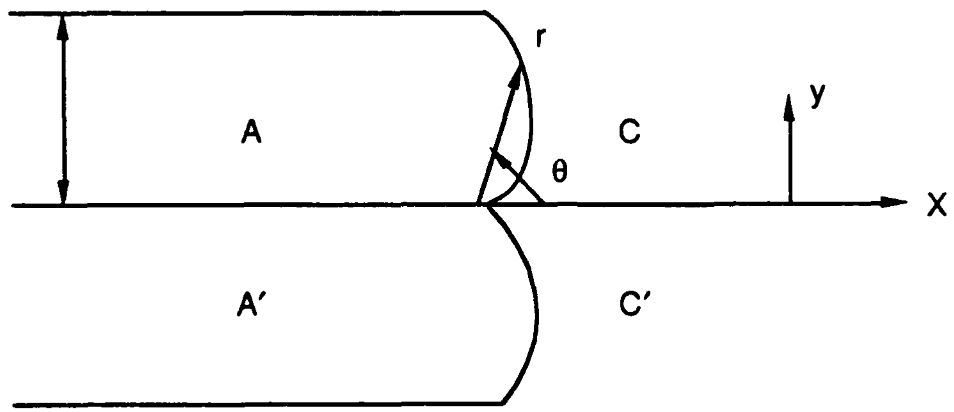
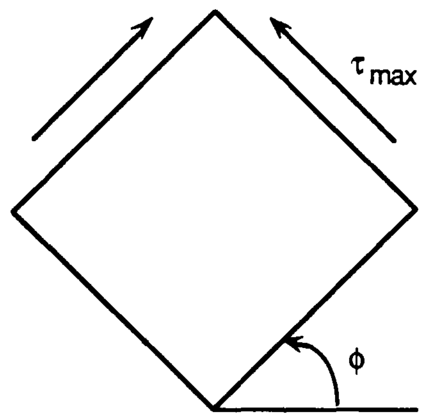


Figure 3.

Along C, $\tau_{max} = \tau_c$, and we will estimate the location of C by calculating τ_{max} only on the basis of the far-field stresses given by the "applied" K. This gives the equation.

$$r = \frac{1}{\pi}\left(\frac{K}{\tau_c}\right)^2 \sin^2\theta \tag{1}$$

for C. The corresponding orientation ϕ of the axes of τ_{max} is (see sketch)



$$\dot{\phi} = \frac{3\theta}{4} \tag{2}$$

The "transformation strains" $\varepsilon^T_{\alpha\rho}$ due to twinning shear strains γ_t along C, oriented according to ϕ, are

$$\varepsilon^T_{11} = \frac{-\gamma_t}{2}\sin\frac{3\theta}{2}$$

$$\varepsilon^T_{22} = \frac{-\gamma_t}{2}\sin\frac{3\theta}{2} \tag{3}$$

$$\varepsilon^T_{12} = \varepsilon^T_{21} = \frac{\gamma_t}{2}\cos\frac{3\theta}{2}$$

If these strains persist in strips in $\pm$ y dy from C to $-\infty$, they induce a change in the stress-intensity factor given by the weight function formula

$$\Delta K = -\frac{E'}{K}\int_C \bar{\sigma}_{\alpha\rho}\,\varepsilon^T_{\alpha\rho}\,dy \tag{4}$$

where $\bar{\sigma}_{\alpha\rho}$ is the applied field, and $E' = \frac{E}{1-v^2}$.

This is the same as

$$\Delta K = -\left(\frac{E'}{K}\right)\tau_c\,\gamma_t\,H \tag{5}$$

where H is the zone height (see Fig. 3).

From (1),

$$H = \left(\frac{1}{8\pi}\right)\left(\frac{K}{\tau_c}\right)^2 \tag{6}$$

so that

$$\Delta K = -\left(\frac{K}{8\pi}\right)\frac{E'\gamma_t}{\tau_c} \tag{7}$$

Also, eliminating (K/τ_c) in (6) we have

$$\Delta K = -E'\gamma_t\left(\frac{H}{8\pi}\right)^{1/2} \tag{8}$$

in terms of the zone height.

The results (7), (8) may now be compared with the available preliminary data (Table I).

TABLE 1

EXPERIMENTAL DATA

Twinning Strain, $\gamma_t^p = 0.707$

Fraction of grains twinned $\cong 0.01$

Zone height, $H \cong 300\mu m$

Critical twinning stress, $\tau_c \cong 70$ MPa

Matrix toughness (no twinning), $K_c \cong 6$ MPa$\sqrt{m}$

Modulus, $E = 200$ GPa

COMPARISON WITH EXPERIMENT

Based on the data [1] in Table 1, Eqn. (7) predicts a toughening $\Delta K_c \approx 13$ MPa$\sqrt{m}$, while Eqn. (8) gives $\Delta K_c \approx 5$ MPa$\sqrt{m}$, compared with a measured value of $\Delta K_c \approx 10$ MPa$\sqrt{m}$. The order of the effect thus appears correct. Further work is needed to provide a refined understanding of the details.

CONCLUDING REMARKS

One important feature to note is that this approach for estimating the influence of mechanical twinning on toughness is applicable when conventional plastic flow also occurs, provided that the plastic zone is much smaller ($\lesssim 1/10$) the size of the twin process zone. Equivalently, the estimate of ΔK_c applies provided that the critical twinning stress τ_c and the shear stress needed for conventional plastic flow, τ_o are subject to the inequality $\tau_c \lesssim (1/3)\tau_o$. The hypothetical stress/strain curve reflecting these requirements is depicted in Fig. 2b.

REFERENCES

1. H. Deve, unpublished research at UCSB.
2. C. Barrett and T. Masalski, Structure of Metals.
3. D. Schechtman, M. J. Blackburn, H. A. Lipsitt, Met. Trans. (1974) 5, 1373.

THE CRITICAL REINFORCEMENT SIZE FOR THE AVOIDANCE OF MATRIX CRACKING

B. Budiansky, A. G. Evans, R. Mehrabian

NOTATION

α_m, α_f	thermal expansion coefficients (matrix, fiber)
E_m, E_f	Young's modulus (matrix, fiber)
ν	Poisson's ratio (assumed the same for matrix and fiber)
f	volume concentration of fibers
R	fiber radius
a	initial flaw size (see Figure 1)
q	radial fiber pressure
σ	circumferential matrix stress (at fiber)
K_m	matrix toughness
ΔT	temperature change
Ω	$(\alpha_m - \alpha_f)\,\Delta T$, thermal mismatch strain

INTRODUCTION

Concepts for enhancing either the creep strength or the ultimate strength or the fracture toughness of intermetallic and ceramic matrices involve the incorporation of fibers, whiskers and/or plates. When these reinforcements have a smaller thermal expansion coefficient than the matrix (a common situation for intermetallic matrices), matrix cracking can occur upon cooling from the processing temperature. The incidence of such cracking can be expressed in terms of a critical reinforcement radius, R_c. The significance of the critical radius is that it represents a bound below which ($R < R_c$) matrix cracking cannot occur. For $R > R_c$ cracking is probabilistic in nature and is governed by details of the flaw populations in the matrix near the interface. For design purposes, R_c represents a fail safe criterion for the assured avoidance of matrix cracking upon processing. For some matrix cracking modes, the applied stress augments the residual stress and causes cracks upon loading. Another critical size for avoidance of cracks upon loading to a specified stress can also be derived.

The types of matrix cracking to be considered are as follows. For aligned fibers and whiskers, both radial and axial matrix cracking are determined. For plates, matrix cracks that form around the perimeter are examined.

ANALYSIS

Aligned Fibers

Radial cracks:

During cooling of an aligned - fiber composite, the thermal mismatch parameter Ω will be positive for $\alpha_f < \alpha_m$, and circumferential tensions will develop in the matrix in the vicinity of each fiber-matrix interface. In the

presence of unavoidable initial flaws in the matrix, cracking driven by these tensions will occur.

A rough but conservative estimate of the condition for cracking can be based on the thermal stresses in the matrix in the absence of flaws. The thermal circumferential tension in the matrix at the interface has been approximated in [1] on the basis of a composite cylinder model by

$$\sigma = \frac{(1+f)\, E_m \Omega}{2(1-\nu) - (1-2\nu)\,(1-f)\,(1-E_m/E_f)} \tag{1}$$

The mode-I stress-intensity factor K at the tip of flaws of length a in the infinite plane configuration of Figure 1 is approximately [2],

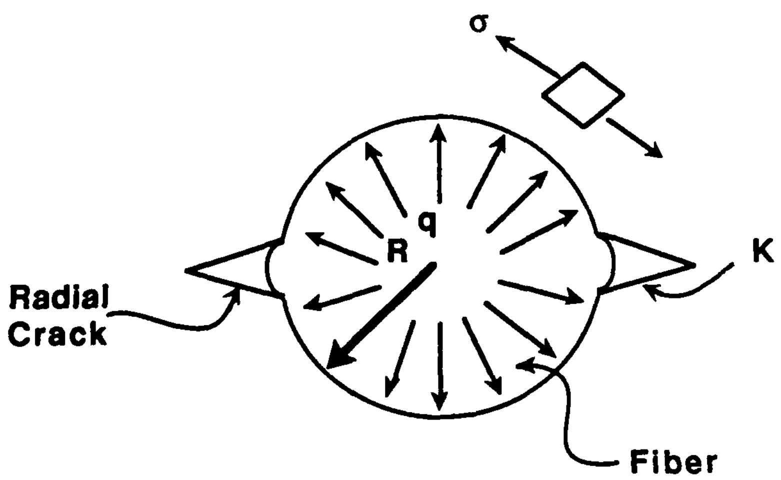


Figure 1.

$$K = \frac{(1.12)\, q\, \sqrt{\pi a}}{1+a/R} \tag{2}$$

In an isolated fiber (i.e., f = o), $\sigma = q$ in the absence of flaws. We propose,

therefore, to replace q in Eq. (2) by the expression (1) for σ for finite fiber concentration. Then, the requirement that $K < K_m$ gives the inequality

$$\frac{\sqrt{B}}{1+B/\eta} < 1 \tag{3}$$

where $\begin{cases} \eta = R/L \\ B = a/L \end{cases}$ (4)

and L is the length parameter

$$L = \frac{4}{\pi(1.12)^2}\left\{\left[\frac{1-\nu}{1+f}\right]\left[\frac{K_m}{E_m\Omega}\right]\left[1-\frac{1}{2}\left(\frac{1-2\nu}{1-\nu}\right)(1-f)\left(1-\frac{E_m}{E_f}\right)\right]\right\}^2$$

Note that (3) is satisfied for <u>all</u> η (hence all R) if $B < 1$. For $B > 1$, we need

$$\eta = \frac{B}{\sqrt{B}-1} \tag{5}$$

This gives a minimum value $\eta_{min} = 4$ for $B = 4$. Hence, there can be no cracking for <u>any</u> flaw size provided that

$$R < 4L \tag{6}$$

or

$$R_c = 4L.$$

For $\qquad E_m \approx E_f$

$$R_c = (4.05)\left[\left(\frac{1-\nu}{1+f}\right)\left(\frac{K_m}{E\Omega}\right)\right]^2 \tag{7}$$

Axial Cracks:

Previous research at the MRC has examined axial cracks [1]. A result of relevance for present purposes is the misfit that causes such cracks when the fiber has a coating subject to debonding and frictional sliding (as exemplified by the C coating on SCS6 fibers). The result for the critical radius is

$$R_c = \frac{3(1-v)^3}{f}(1+v)\ \mu \left(\frac{K_m}{E\Omega}\right)^2 \tag{8}$$

where μ is the friction coefficient ($\mu \approx 0.1$ to 0.2 for C debond coatings). It is important to note that for reasonably high fiber volume fractions ($f \approx 0.4$), R_c for axial crack is smaller then that radial cracks when μ is relatively small.

Axial cracks, suppressed upon processing, can form during loading, yielding another critical radius,

$$R_c' = \frac{R_c}{[1+(1-v)\ \sigma/E_f\Omega]^3} \tag{9}$$

where σ is the expected axial stress.

In the absence of sliding ($\mu \rightarrow \infty$), another bound has been derived [1]. This solution gives a critical radius.

$$R_c = \frac{1.5\ (1-v)^2}{(1+v)^{1/2}\ f\ \ (1-f)} \left[\frac{K_m}{E\Omega}\right]^2 \tag{10}$$

PLATES

Plate-shaped reinforcements subject to positive misfit, Ω, exert a large tensile stress concentration on the matrix around the plate perimeter (Fig. 2). A small flaw located in this region converts the configuration into a crack-like entity, with pressure P acting over the segment, 2R. The stress intensity factor is;

$$\frac{K}{p\sqrt{R}} = \frac{2}{\sqrt{\pi}}(1+\lambda)^{1/2}\left[1 - \sqrt{1 - 1/(1+\lambda)^2}\right] \tag{11}$$

where $\lambda = a/R$. This has its maximum value at $\lambda = 0$, given by,

$$\frac{K_{max}}{p\sqrt{R}} = \frac{2}{\sqrt{\pi}} \tag{12}$$

For an isolated ellipsoidal plate, the normal pressure p has the form,

$$p = \frac{2}{3}\frac{E\Omega A}{(1-v)} \tag{13}$$

where A is an unknown function of the aspect ratio (A will be calculated soon).

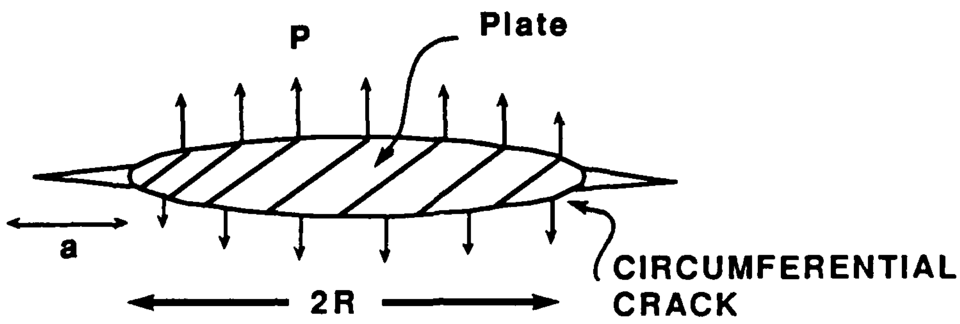


Figure 2.

Putting $K_{max} = K_m$ and combining Eqns. (12) and (13), the critical radius a is derived as;

$$R_c = \frac{9\pi}{16}\frac{(1-v)^2}{A^2}\left[\frac{K_m}{E\Omega}\right]^2 \tag{14}$$

Note that $2R_c$ is the major dimension of the plate. The influence of volume fraction f on the critical size is not as readily calculated, but the effect is expected to be small for $f \lesssim 0.2$.

SOME TYPICAL RESULTS

The implications of the above calculations are illustrated for two important intermetallic systems reinforced with ceramics: γ–TiAl and $MoSi_2$ reinforced with either SiC or Al_2O_3. Thermal expansion information for these materials is shown in Figure 3. Other known properties are listed on Table 1. To facilitate the analysis the above calculations are first plotted as a function of volume fraction on Figure 4. It is evident that the preference for axial or radial cracks in fiber composites is dominated by the friction coefficient, μ. For C coatings on SCS6, this coefficient is believed to be ~0.1. With this choice, critical radii evaluated for a volume fraction f = 0.4 are summarized in Table II (ΔT is ~1000°C for γ–TiAl and ~1300°C for $MoSi_2$). It is recalled that R_c for the plate refers to their major dimension whereas R_c for the fibers refers to this minor dimension.

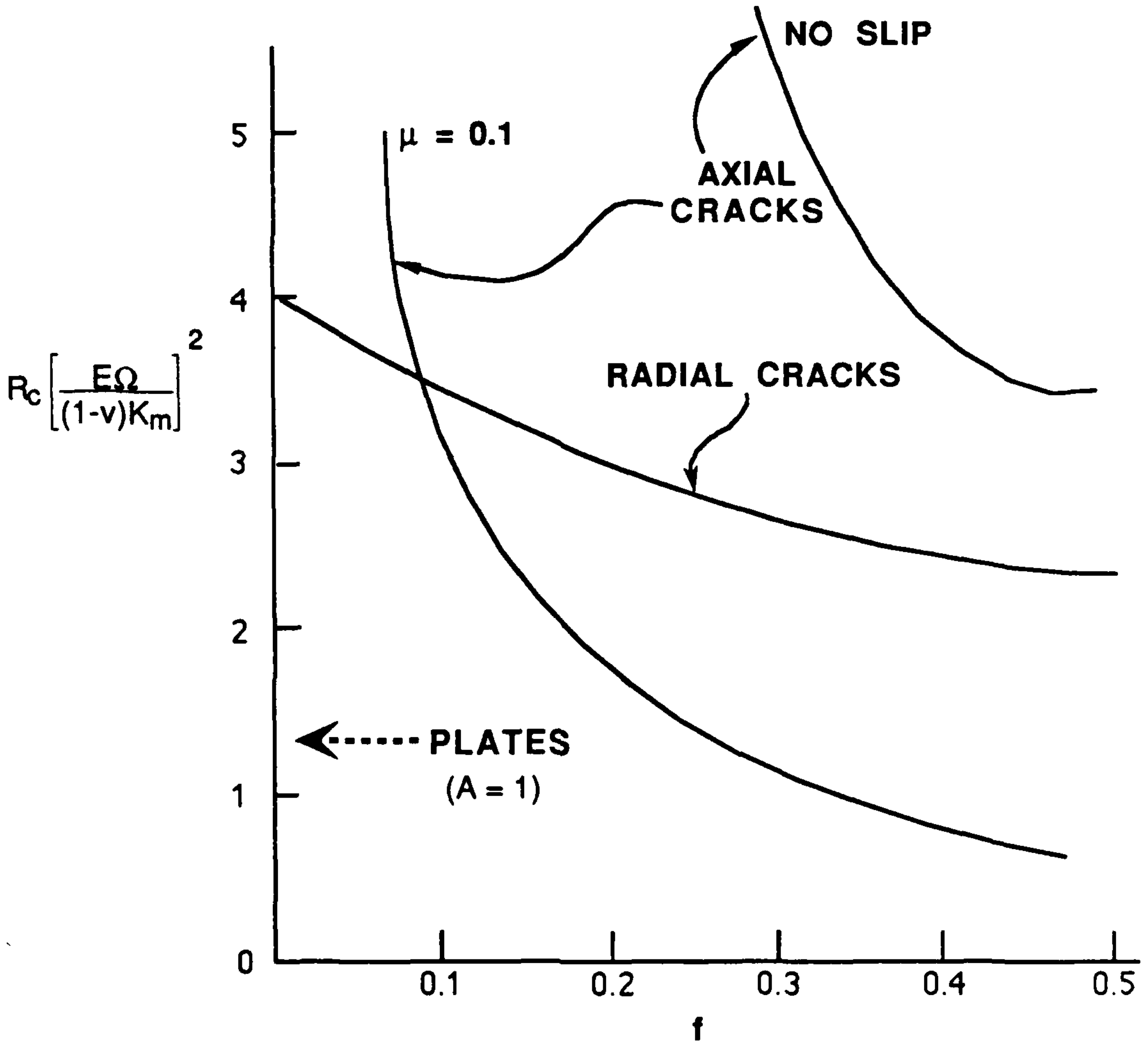

NO SLIP
AXIAL
CRACKS
μ = 0.1
RADIAL CRACKS
PLATES
(A = 1)
$R_c \left[\frac{E\Omega}{(1-\nu)K_m}\right]^2$
5
4
3
2
1
0
0.1
0.2
0.3
0.4
0.5
f

Figure 4.

TABLE I

MATERIAL PROPERTIES

MATERIAL	$E(GP_a)$	v	$K_m(MPa\sqrt{m})$
γ-TiAl	250	0.3	6-8
$MoSi_2$	380	0.3	5-6
SiC	420	0.2	2-3
Al_2O_3	420	0.2	3-4

TABLE II

CRITICAL RADII (in MICRONS) (f = 0.4)

MATERIAL COMBINATION	ALIGNED FIBER			PLATES*
	AXIAL ($\mu = 0.1$)	NO SLIP	RADIAL	
TiAl/SiC	3	12	8	7
$TiAl/Al_2O_3$	6	24	16	14
$MoSi_2/SiC$	5	20	12	11
$MoSi_2/Al_2O_3$	200	400	450	400

*Approximation for A = 1.

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2. Tada, P. Paris and G. Irwin, Handbook of Stress Intensity Factor, Del Research (1973).

ADVANCED COMPOSITES WITH IMPROVED COMPRESSIVE PROPERTIES

J. Economy

INTRODUCTION

Composite structures based on high modulus/strength graphite or Aramid fibers share a common shortcoming namely their modest to poor compressive properties. This problem appears to be related to the morphological features of these fibers since boron and even glass fiber composites perform far more effectively under compressive forces. This drawback has greatly limited a broader usage of these fibers since structural composites must be capable of withstanding a wide range of complex forces among which compression is one of the most critical. Although this problem has been recognized for many years there has been little or no progress made on improving this property or even in establishing the root causes. The complexity of the problem is illustrated by the fact that some improvement in compressive properties of graphite composites has been realized using thermoplastic matrices although the reasons are not particularly obvious. However, this merely serves to indicate that a meaningful program on improved compressive properties will require better understanding of the respective roles of the fiber structure and morphology, the matrix and the fiber matrix interface.

DISCUSSION

In this section the various factors which might contribute to the poor compressive properties are considered and then approaches proposed to address these problems.

Fiber Structure & Morphology

The features which distinguish graphite and Aramid fibers (includes PBO & PBS fibers) from all other reinforcing fibers are the microfibrillar structure and the variation in structural anisotropy across the diameter which can result in a skin-core effect (surface being most highly oriented). Both of these features have their origins in the early stages of filament processing. Thus, skin-core effect is due to the high chain orientation which arises at the surface of the spinnerette hole in the spinning of the polyacrylonitrile precursor (PAN) or the Aramid solution. Since the thermal expansion coefficient (TEC) of the surface is lower than that of the core, the surface is placed under compression while the core is under tension. These forces are sufficient that in melt processing liquid crystalline polymers under high shear conditions the surface tends to delaminate from the core. The microfibrillar structure is typically observed in a wide range of melt and solution spun organic fibers and its origins are not particularly clear. However, it would appear reasonable that the lateral forces between the microfibrils are relatively low and transfer of load in flexure or compression is sharply compromised. Another structural feature shared by the graphite and Aramid fiber is the absence of three dimensional order within the microfibril. Thus in graphite fiber the layered structure is turbostratic, i.e., the hexagonal layers are not registered while in the Aramids the rod like chains pack tightly but there is no three dimensional order. It is noteworthy that fibers which display reasonably good compressive properties such as boron or even glass do not have a microfibrillar structure nor do they display the skin-core effect.

There are several approaches which could be pursued to distinguish the respective roles of the microfibrillar structure, skin-core effect and the absence

of three dimensional order. With respect to the microfibrillar structure one could pass the Aramid fiber or graphite fiber precursor through electrically heated rolls above their plastic deformation temperature to permit fusion between the microfibrils. Although one would also deform the fibers into ribbons this should be of little concern in evaluating the effect on compressive properties in composites. This kind of process may also act to somewhat minimize the problems associated with the skin-core effect.

An alternative approach for directly addressing the skin-core and microfibrillar problems at the same time would be through the study of high modulus/strength BN fibers. These fibers resemble graphite fibers in most ways including the turbostratic structure and ability to stress graphitize to achieve very high mechanicals. The BN fibers are prepared by chemically reacting a B_2O_3 precursor fiber with NH_3. Because of the isotropic nature of the B_2O_3 glass there is no tendency to form either a microfibrillar or skin-core structure.

Although considerable work was done in this area by the PI in the early 1970's, no data was generated on composite properties and particularly those in compression. Hence, if any BN fibers are still available it would be of great interest to determine their compressive properties. Otherwise, it would be important to prepare small samples for fabricating test bars. One minor change that would be made is to incorporate small amounts of SiO_2 into the B_2O_3 glass. During subsequent processing the SiO_2 will accumulate in the grain boundaries and at the fiber surface to facilitate bonding to resin matrices and to further stabilize the BN to oxidation at temperatures in excess of 850°C.

A third approach which is already under investigation by the author is to prepare single crystal fibers of poly p-hydroxy benzoic acid or poly-2, 6-hydroxy-naphthoic acid. Both of these material display an unusual propensity

to polymerize into single crystal structures. In addition they each melt into a liquid crystalline phase at 450°C which should permit formation of continuous melt drawn filaments. During the melt spinning and drawing process the polymer chains in the fibers would tend to lock into a three dimensional ordered structure because of the strong ester-ester dipolar interactions. Presumably such forces would be sufficient to overcome the tendencies to preserve the elongated domain structure of the liquid crystalline melt which may very well be the cause of the microfibrils and the skin-core effect.

The Fiber Matrix Interface

The mismatch in TEC between the matrix and either graphite or Aramid fiber presents a major problem in optimizing the mechanical properties of these composites. The problem is further exacerbated by the fact that both the carbon fiber and Aramid fiber surfaces display the highest degree of orientation and consequently the lowest TEC. Presumably a matrix which effectively matched the low TEC of the fiber at the interface and then displayed a gradation away from this surface to a more isotropic state could provide a unique solution to this problem.

One approach to designing a matrix which would match the TEC of the fiber at the interface is through use of liquid crystalline polyesters. In fact, such a concept was described several years ago in the literature by Celanese researchers, however, they were unable to observe any measurable improvement in reinforcing. One of the problems in their approach was the use of the high Mn copolyester of p-hydroxy-benzoic acid (PHBA) and 2, 6 - hydroxynaphthoic acid (PHNA). Because of its relatively high viscosity (especially with little or no applied shear) the ability to flow into the fiber interstices, wet the surface and then undergo some morphological orientation at

the interface to match the fiber TEC would be greatly limited. Hence it is not surprising that the Celanese work was rather discouraging with respect to this concept. Alternatively, if one were to use a low Mn (~2000) precursor liquid crystalline polyester the above problems would be greatly reduced. Thus the much lower melt viscosity of the precursor would permit effective wetting of the fiber surface at relatively low temperatures of 200-280°C and the potential to self orient at the fiber surface during cooling. Prepregs could then be advanced to Mn ~10,000 which involves evolution of several percent gas in the form of end group. Initially a prepolymer from the copolymerization of PHBA & PHNA would be evaluated because of its ease of processibility. With any success in this approach, the effort would be shifted to the prepolymer of PHBA with biphenol terephthalate (BPT) since the latter system would permit a composite use temperature of 350°C as opposed to 120°C for the PHBA/PHNA copolyester.

Matrix

Some of the considerations concerning the design of an improved matrix for graphite and Aramid composites have already been discussed in the previous section. Suffice it to say that for improved composites, one should strive to design tough matrices with sufficient crosslinking to maintain high mechanicals at elevated temperatures in excess of 300°C.

One approach that would be pursued in this program is to develop branched polyesters with carboxylic acid end groups. When heated to over 350-400°C these polyesters would undergo rapid interchain transesterification to yield a three dimensional network. These interchain transesterification reactions have recently been shown by the author to occur at a rate 1000 ester

interchanges per chain every ten seconds at 450°C. The advantage of such a system is that crosslinking can be designed to take place without evolution of any volatiles. Furthermore, at 350°C the thermal oxidative stability is outstanding and up to 50% of the mechanical properties are retained. A preferred process for graphite fibers would be to initially coat the fiber with a prepolymer of PHBA/BPT and then add a second prepolymer from a branched polyester using the 1,3,5- tricarboxylic acid of benzene and PHBA. Both prepolymers could be advanced by heating to 350°C still in the form of a prepreg. The desired structure would be formed by stacking the laminates and briefly heating at 200 psi at 400-450°C to effect the rapid interchain transesterification to a crosslinked structure.

COATINGS FOR FIBER REINFORCED INTERMETALLICS

R. Mehrabian, A. G. Evans, W. Barker

COATING REQUIREMENTS

Coating concepts applicable to fiber reinforced intermetallics have been identified based on available information about phase compatibility, thermal expansion and debonding/sliding. The discussion focused on $MoSi_2$, γ-TiAl, $TiTaAl_2$. TiAl is regarded as a material with potential up to 900 to ~1000°C, $TiTaAl_2$ as a 1000 to ~1200°C material and $MoSi_2$ as potentially capable of >1200°C.

Creep data on fine grained polycrystalline Al_2O_3 indicates that this material behaves as a superplastic solid having creep rate governed by the Sherby parameter,

$$\frac{\dot{\varepsilon}\, d^3}{D_b \delta_b} \sim (\sigma/\mu)^2 \tag{1}$$

where $\dot{\varepsilon}$ is the strain-rate, d the grain size, $D_b\delta_b$ the grain boundary diffusion parameter, σ the stress and μ the shear modulus. Based on creep data obtained on Al_2O_3 at 1200°C and knowing the temperature dependence of $D_b\delta_b$, it is apparent that submicron grain size Al_2O_3 fibers are expected exhibit substantial creep at temperature above 1000°C. Indeed, Al_2O_3 would be more prone to creep than $MoSi_2$. It was thus concluded that polycrystalline Al_2O_3 fibers could be generally used for toughening purposes, but are only useful for creep strengthening of γ-TiAl and possibly $TiTaAl_2$ up to ~1000°C. This background leads to the fiber reinforcement suggestions indicated on Table I.

This list is based on present experience and is not intended to be inclusive, but provides a focus for the next set of experiments on both laminates and actual composites.

COATING APPROACHES

The use of CVD methods to provide thin (~0.1μm), uniform coatings on fiber tows has been extensively explored at 3M by Tom Gabor. Remarkable flexibility and control have been demonstrated. Examples of coatings already produced on Nextel fibers are presented in Table II. A match between this capability and the above requirements can be envisaged and should be exploited.

SPECIMEN TESTING

The coating concepts presented in Table I can be explored by testing both laminates and actual composites. For the laminate approach, a sapphire disc ~1 inch in diameter must be coated and then bonded to matrix plates in a sandwich configuration. A portion of the plates can be used for diffusion couple tests. Also, tension tests may be performed and cracking in the sapphire monitored by optical microscopy. The interaction of these cracks with the coating, including the evolution of debonds will provide the required information about the mechanical characteristics of the coatings.

A second test approach requires the incorporation of coated fibers into the matrix of interest, followed by flexural testing to measure the work of fracture.

A third approach is to introduce single crystal α-SiC dissipates in with the aluminide and silicide matrices. Preliminary calculations show that plate diameters should be less than ~10μm for both matrices in order to avoid matrix cracking due to thermal mismatch strains. Nevertheless, preliminary

experiments should be undertaken, perhaps in the $MoSi_2$ matrix, to test the possibility of both creep and toughness (coated SiC plates) improvements. It should be noted that α-SiC single crystal plates are expected to retain significant strengths up to ~1500°C.

TABLE I

Coating Preferences For Fiber Reinforced Intermetallics

i) 1000°C to 1200°C, use → γ-TiAl and $TaTiAl_2$

PROPERTY	FIBER	COATINGS	
		PROTECTIVE	DEBOND
TOUGHNESS	Al_2O_3*	Y_2O_3	Mo
		YAG	$MoSi_2$
		TiB_2	Ir
		AlN	Pt
CREEP	SAPPHIRE**	Y_2O_3	NONE

* $\Delta\alpha$ for SiC too large for fibers $\gtrsim$ 3 to 8μm

** Creep of polycrystalline Al_2O_3 may be too large above ~1000°C

ii) $\gtrsim$ 1200°C use → $MoSi_2$ Matrix

PROPERTY	FIBER	COATING	
		PROTECTIVE	DEBOND
TOUGHNESS	Al_2O_3	TiB_2 NONE !	? SiC
	W	Al_2O_3	?
CREEP	SAPPHIRE	NONE	NONE
	W		

TABLE II

SINGLE COATING

	EXPL.	COLOR	ELECTRICAL RESISTANCE (kΩ/m)	STRAND STRENGTH (kg)	DEV. (%)	BEND STRENGTH (kg)	DEV. (%)
1.	SiC	golden	∞	2.4	-33	0.3	-92
2.	AlN	*grey	9000	3.9	-30	1.6	-48
3.	BN	straw	∞	4.2	- 4	3.2	- 4
4.	BN	straw	∞	3.2	-27	3.0	-12
5.	B_4C	black	$3x10^4$	1.7	-64	1.0	-74
6.	C	black	76	4.2	- 5	3.6	7
7.	Mo	black	2.4	4.7	-16	2.7	45
8.	$MoSi_2$	black	400	4.1	-28	1.9	2
9.	SiO_2	white	∞	2.9		2.2	-30
10.	Si_3N_4	white	∞	1.2		1.2	
11.	SnO_2	*golden	32	1.9	-56	0.0	
12.	SnO_2	white	10	2.2	-48	0.5	-86
13	SnO_2	black	32	3.1	-36	0.5	-91
14.	SnO_2+F	*olive	2.4	1.8	-57	0.0	
15.	SnO_2+F	white	10	2.1	-51	0.5	-81
16.	SnO_2+F	black	1.4	4.2	-15	0.5	-86
17.	Ta_2N	black	5.6	5.9		1.7	- 7
18.	TiB_2	black	8.0	5.9	28	2.8	-30
19.	TiB_2	black	4.0	4.9		0.7	-70
20.	TiN	black	170-6700	2.6	-52	1.0	-75
21.	TiN	golden	1.1	0.0		0.0	
22.	ZrN	olive∞	5.1		1.8		
23.	ZrO_2	white	∞	3.8	-20	3.2	10

MULTIPLE COATINGS

24.	AlN/BN	grey ∞	4.5	- 3	2.4	-34	
25.	C/BN	black	28	5.6	21	2.7	-32
26.	SiC/BN	golden	∞	4.2		1.3	-59
27.		golden	∞	4.2	-21	2.4	-11
28.	SiC/C	black	160	3.2	-27	0.8	-75
29.	Si_3N_4/BN	white	∞	1.2		1.2	
30.	SnO_2/BN	*golden	36	2.0	-25	0.5	-84
31.	SnO_2+f/BN	olive	1.4	2.3	- 7	0.5	-84
32.	TiB_2/C/BN	black	4.0	4.6		3.0	
33.	TiC/BN	black	6.0	5.4	-10	4.4	76

COMPOSITE COATINGS

34.		*grey	∞	4.5	-12	3.1	35
35.	SiC-TiC	grey	1×10^4	7.6	-25	1.7	-68

INTERATOMIC POTENTIALS

H. Ehrenreich, J. Hirth and D. Srolovitz

INTENT

- Review the status of Interatomic Potentials for Atomic Modeling by Computer Simulation.
- Stress the relevance of modeling defects and structures of a size scale inaccessible to microscopy.
- Emphasize the importance of linking continuum and atomistic descriptions of solids, and of the relevant scientific communities.

EXECUTIVE SUMMARY

The status of interatomic potentials used for atomic simulations of structures and structural defects in solids was assessed in a one-day meeting. Problems of importance to DARPA involve defect configurations that, at present, cannot be experimentally probed. These include properties related to deformation (dislocation core structure, extended dislocation arrays, dislocation motion), fracture (lattice trapping, crack propagation, dislocation emission from cracks), diffusion (particularly at low temperatures and small distances as in VLSI structures), and grain boundaries and interfaces (energies, impurity effects, grain boundary separation). Such defects can be simulated by microscopic atomistic calculations and can be used predictively provided that the interatomic potentials for modeling inter-atomic interactions in real materials are reliable.

Simple empirical pair-potentials have been used to describe these interactions over three decades. However, it has been evident that such

potentials are poor in describing open crystal structures and free surfaces. Some pair potentials were modified, early on, by adding a phenomenological volume-dependent term. Recently, other methods have been developed to include many-body interactions contained in this volume-dependent term systematically. In the case of metals, the "embedded atom method" (EAM) and the "equivalent crystal method", among others, yield potentials having a similar formal structure. They include a pair-type interaction and a term depending on the perturbed electron density in the neighborhood of the defect. For covalent crystals such as silicon, angularly dependent pair-type interactions effectively lead to directional bonding.

These methods have yielded good results for surface and stacking fault energies in metals as compared to both experiment and ab initio calculations using the LDA methodology. In some cases, for example intermetallic compounds, better fits to experimental data were achieved using EAM potentials and fitted empirical constants. In silicon good agreement between theory and experiment was obtained for elastic constants, phonon frequencies and a variety of defect energies. These results indicate that this approach towards modelling the properties of complex defects in solids realistically is promising and deserving of further development.

A meeting highlight concerned the remarkable correlation found by J. Smith and coworkers in the form of a universal energy-interatomic separation curve that applies to cohesion, surface adhesion, and chemisorption of a wide variety of materials (e.g., Mo, K, Cu, Ba, Sm and non-metals like Si). The fit to experimental quantities involves a simple empirical expression for the energy containing just a single energy and a single distance parameter. This correlation serves to motivate the search for general interatomic potentials of

the sort described here. There is little understanding of the fundamental basis of this correlation. Further insight would benefit the search for better interatomic potentials considerably.

VIEWGRAPH SUMMARY

1. Defines pair potentials and embedded atom-type potentials. These consist of two terms, a pair potential term, and a volume dependent many-body term that depends on the local electron density at the defect site.
2. Lists atomic simulations that have impact on materials properties. The effects of particular types of defects which are inaccessible to experiment or first principles calculations because of their complexity requires understanding in the design of materials having specified properties.
3. Lists the presently available results from pair potentials and embedded atom-type potentials and their characteristics. Pair potentials have limited applicability because they are qualitative. The more complicated potentials are more quantitative and tend to be insensitive to the details of the potential. They show promise of predictability, but thus far the results obtained are relatively few in number.
4. A figure, due to J.R. Smith, gives the basis underlying the "universal" binding energy $E^*(a^*)$ curve. The scaled energy E^* and lattice parameter a^* are defined on the figure. The wide applicability of scaling to chemisorption, adhesion, and cohesion in metals is illustrated, as is the fact that this viewpoint is also applicable to something as simple as a H_2^+ module.
5. Illustrates the universal binding energy relation for metals. Remarkably, each property shown for a variety of materials, falls on the <u>same</u> $E^*(a^*)$ curve. The reason for this behavior remains to be understood.
6. States the relevance to DARPA interests.
7. Presents a summary. Clearly further work in elucidating the reasons for the apparent "universal" behavior, and calculations of other defect properties using the new interatomic potentials needs to be performed. Support of

such research is in DARPA's interest. However, other agency funding would be equally appropriate.

INTERATOMIC POTENTIALS

Pair Potentials

$$\text{Energy} = \frac{1}{2}\sum_{i,j} V(R_{ij})$$

$V(R_{ij})$ = pair potential of two atoms located on sites i and j, separated by distance R_{ij}

Embeded Atom-Type Potentials

$$\text{Energy} = \frac{1}{2}\sum_{i,j} V(R_{ij}) + U_N$$

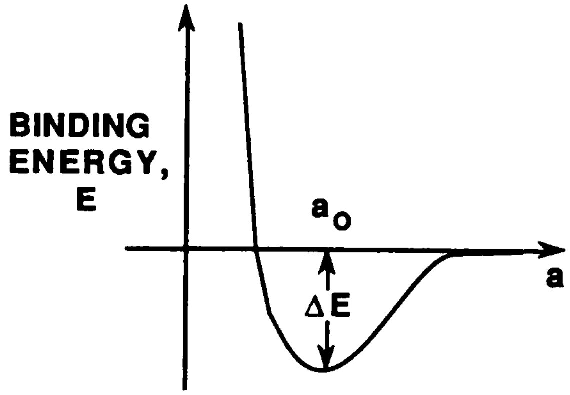
U_N = N-body volume dependent potential = $\sum_i F(\rho_i)$

$F(\rho_i)$ = physically determined function of

$\rho_i = \sum_j \rho_i^a (R_{ij})$ = "local" electron density

ρ_i^a = atomic charge density

Tight binding: $F(\rho)\ \alpha \sqrt{\rho}$



$$E(a) = \Delta E \;\; E^*(a^*)$$

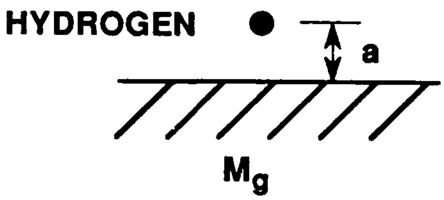
$$a^* = \frac{a - a_o}{l}$$

$$l = \left[\frac{\Delta E}{\left(\frac{d^2 E(a)}{d a^2} \right)_{a_o}} \right]^{1/2}$$

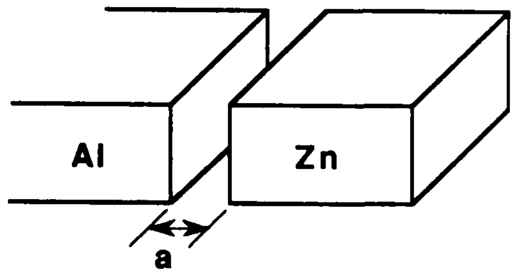
Is $E^*(a^*)$ universal?

Metals:

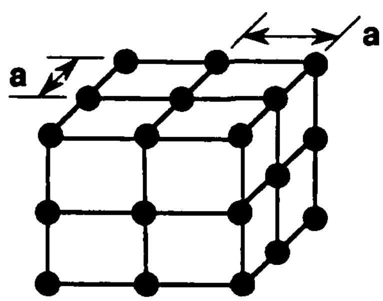
- Chemisorption



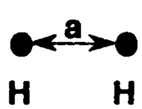
- Adhesion



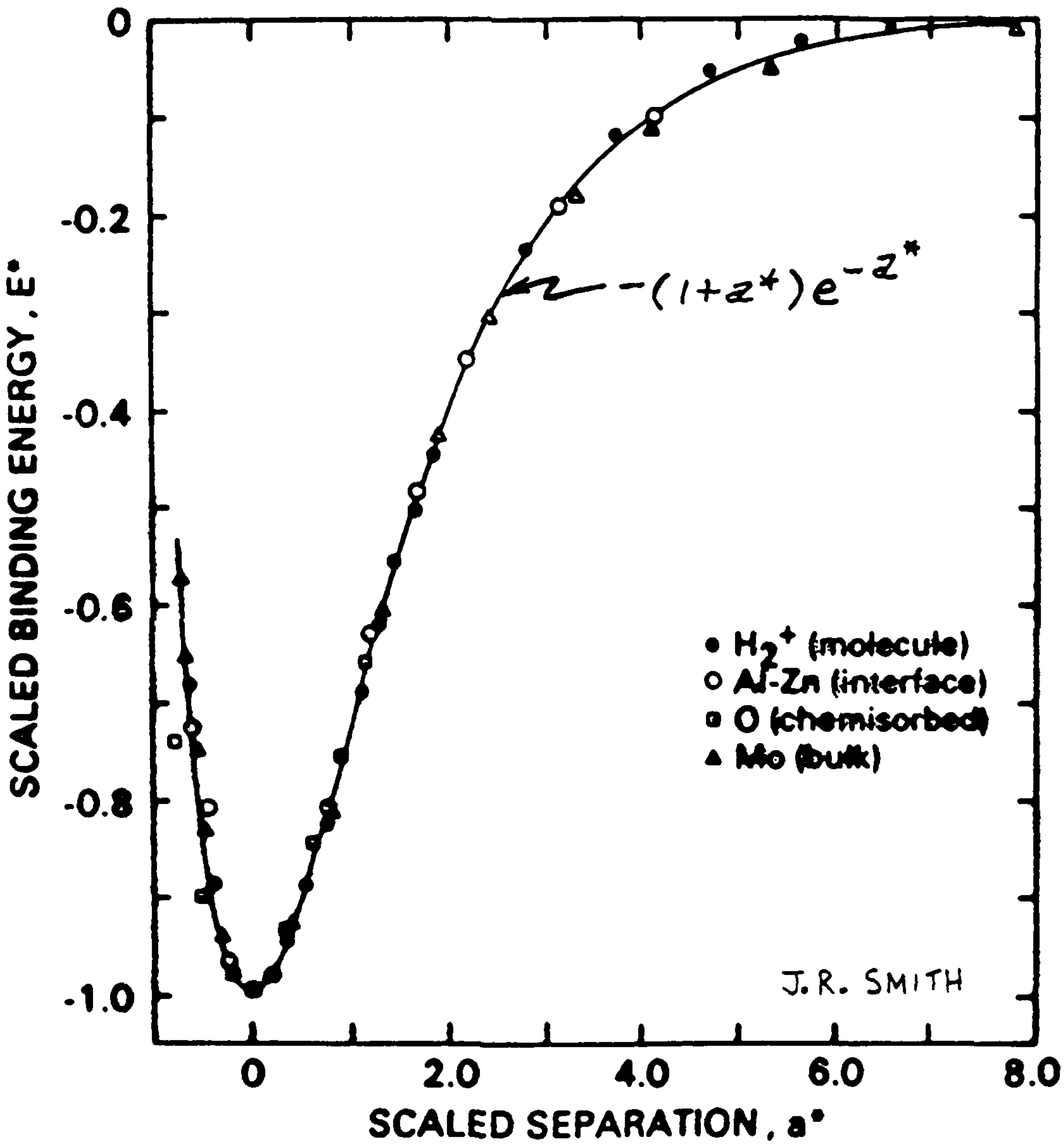
- Cohesion



Diatomics:



UNIVERSAL BINDING ENERGY RELATION FOR METALS



ATOMIC SIMULATIONS WITH IMPACT ON MATERIAL PROPERTIES

- **Deformation**

  Dislocation Core Structure

  Extended Dislocation Arrays

  Dislocation Motion

- **Fracture**

  Lattice Trapping

  Crack Propagation

  Dislocation Emission from Cracks

- **Diffusion**

  Effect on VLSI Structures

AVAILABLE RESULTS

- **Pair Potentials**

  Results: Qualitative, Potential dependent, Limited Predictability.

  -Dislocation Core Structure

  -Interfaces: Grain Boundaries, Stacking Faults

  -Phase Diagrams

  -Nucleation

  -Radiation Damage/Collision Cascades

- **Embedded Atom-Type Potentials**

  Results: Quantitative, Potential Insensitive Some Predictability, Limited in Extent.

  -Complex Crystal Structures

  -Surface Structures and Energies

- **Can Predict Atomic Structure and Energy of Cu, Ag, Fe Surfaces to 0.01 A and 10% Relative to First Principles Values.**

RELEVANCE TO DARPA INTERESTS

- Simulations of cracks, dislocations, etc.

  $\Downarrow$

  Micromechanics/Design Parameters of Composites, other Microstructures that cannot be experimentally determined.
- Kinetic processes, e.g., crack tip propagation, small-scale diffusivity at low temperatures, inaccessible to experimental determination, can be simulated.

SUMMARY

- New interatomic potentials, including many-body effects, yield improved description of crystal structures, surface properties and defect energies of metals and semiconductors.
- These potentials can be used with increased confidence to simulate structural defects inaccessible to experimental observation or first-principles calculations.
- The "universal" correlation between scaled energy and atomic spacing discovered by Smith provides rationale for the notion of a generally applicable interatomic potential.
- The reasons for the universal correlations need to be understood.

AGENDA AND PARTICIPANTS:

AGENDA
INTERATOMIC POTENTIALS
July 17, 1989

OBJECTIVE:

To consider the current status of interatomic potentials for atomic modeling by computer simulation and future prospects for improvements.

ORGANIZERS: Henry Ehrenreich and John Hirth

Monday, July 17 Session I Chairperson: H. Ehrenreich

Overview of Atomic Potentials - A. Carlsson, Washington University

Embedded Atom Method - Murray Daw, Sandia Corp.

Empirical Interatomic Potential for Covalent Systems - Jerry Tersoff, IBM Watson Res. Ctr.

Session II Chairperson: J. P. Hirth

Surfaces and Interfaces - John Smith, GM Research Labs.

Discussion: Speakers, M. Eberhart (LANL) and Council Members

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REFRACTORY COMPOUNDS

J. P. Hirth, R. Mehrabian, B. A. Wilcox

EXECUTIVE SUMMARY

A one day session was held to assess high temperature refractory compounds for use in the 1000-1400°C temperature range for turbine engines and aerospace structures. Lighter alloys are needed for the lower end of this temperature range, e.g., for compressor components in the engine and external skins of high Mach number aircraft. On the other hand, projected turbine temperatures are well above current operating temperature of Ni-base super-alloy components. The payoff for such materials would be increased performance, smaller size/decreased detection probability, and increased payload in advanced aircraft. Current efforts have focussed on ductile refractory alloy and intermetallic matrices with possible fiber reinforcement. Also of potential interest but less studied are beryllide matrices with substantially lower densities. The important properties to be achieved are low density, toughness at low and intermediate temperatures, ductility at intermediate temperatures, creep strength at elevated temperatures, environmental resistance and thermal expansion compatibility. Of the current alloys, Ta-Ti-Al alloys with Y or Hf additions for enhanced oxidation resistance show the most promise among a number of ductile refractory compounds. For these alloys, concepts of microstructural phase distribution design are being incorporated to fine tune the properties. Extensive fundamental work is underway to couple the ternary phase diagram modeling with calculation of solidification "paths" to produce desired microstructures. Examples were given for both the Ta-Ti-Al and

Nb-Si-Al systems. Since oxidation is a major concern at these high temperatures, production of equilibrium microstructures prior to service is important. Consequently, reduced segregate spacing, i.e., through rapid solidification, is desirable due to slow diffusion in these alloys at temperatures below that for aluminum volatilization. Enhanced creep performance through the introduction of coarse, long aspect ratio, second phases, e.g., borides, is also under study. Finally, coatings are needed to prevent oxidation and interstitial pickup.

The compound $MoSi_2$ appears to have the best properties, especially oxidation resistance, among the silicides studied to date. With SiC whisker reinforcement, the mechanical properties at high temperature are good. Aluminum or germanium additions prevent the "pest" oxidation at intermediate temperatures and the high temperature oxidation resistance under static exposure is adequate. However, the silicaceous natural coating flows above about 1300°C so problems could arise under dynamic exposure and further coating research is required. The ductile-brittle transition temperature is in the 850-1000°C range. While designers are willing to accept limited ductility at room temperature, intermediate, 400-500°C, ductility/toughness is required, so work to decrease the DBTT is also needed. Compositing approaches to be investigated include introduction of coarse particulates, coated fibers and ductilizing phases.

Several transition metal beryllides, for example $ZrBe_{13}$ and $NbBe_{12}$, have very large specific strengths at 1000-1200°C because of their low densities. Work is just beginning at several laboratories to evaluate the potential of such alloys. Older work on low-purity beryllides show DBTT's in the range of 1100°C so work on toughening is needed. Also, BeO reacts with water

vapor to form a volatile hydroxide above about 1000°C and coating will probably be required for resistance to environment effects. Hence, the problems that require study for the beryllides are parallel to those needed for $MoSi_2$.

The alloy development groups working on these materials are beginning to incorporate processing/microstructual design/micromechanics concepts developed under the DARPA/URI Brittle Matrix Composites program. It would be beneficial if continued contacts on a semi-annual basis between the development groups and the Composites Research Group could be facilitated.

APPENDIX: Summary Viewgraphs

The following figures illustrate the potential of the refractory compounds for elevated temperature use. The creep comparison in Figure 1 shows that several of the ductile refractory alloys and $MoSi_2$ have adequate creep resistance for use at temperatures near 1200°C. Figure 2 shows a fiber strengthening structure optimized on the basis of micromechanics alloy design. The structure features a system with matched thermal expansion properties; fiber coating both to prevent fiber/matrix interaction and to provide interface decohesion at a crack tip leading to fiber pullout to enhance toughness; and whiskers/platelets dispersed in the matrix to enhance strength and creep resistance at elevated temperatures. Figure 3 shows an example of long aspect ratio borides in a Ti-Al-Ta matrix produced by a sequential solidification process. Note the stability of these microstructures after heat treatment at 1200°C. Figure 4, specific strength versus temperature, illustrates the reason for the interest in beryllides. The final viewgraphs, Figures 5 and 6, summarize

the status of research and development and recommended action for DARPA for the refractory compounds.

REFRACTORY COMPOUNDS
AGENDA
JULY 18, 1989

OBJECTIVE:

To review processing/microstructure/properties of refractory compounds and establish guidelines for microstructural design on the basis of micromechanics models.

ORGANIZERS: John Hirth, Robert Mehrabian and Ben Wilcox

Tuesday, July 18 Session I Chairperson: J. Hirth

Nb and Ta Alloys and Compounds for High Temperature applications	R. Hecht, Pratt & Whitney Aircraft
Solidification Processing and Composites of Nb-Si-Al alloys and Compounds	R. Mehrabian, UCSB/MRC
Processing, Microstructure, and Properties of Be Alloys and Beryllides	L. Jacobsen Los Alamos National Lab.

Session II Chairperson: R. Mehrabian

Microstructure and Mechanical Properties of Nb-Be Compounds	S. Bruemmer, Battelle Pacific Northwest Lab.
Creep Properties of TiAi/TiB2 and MoSi2 Structures	P Martin, Los Alamos National Lab.
Development of a Reliable Fabrication Technique to Produce Intermetallic Compounds	W.C. Moshier Martin Marietta Space System Denver, Co.

Discussion

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REFRACTORY COMPOUNDS

J. P. Hirth, R. Mehrabian, B. A. Wilcox

Refractory Compounds

Processing/Microstructure/Properties

Micromechanics/Microstructural Design

Relevant to Advanced Aerospace Structures and Engine Components for High Mach Number Aircraft and High Temperature Operation

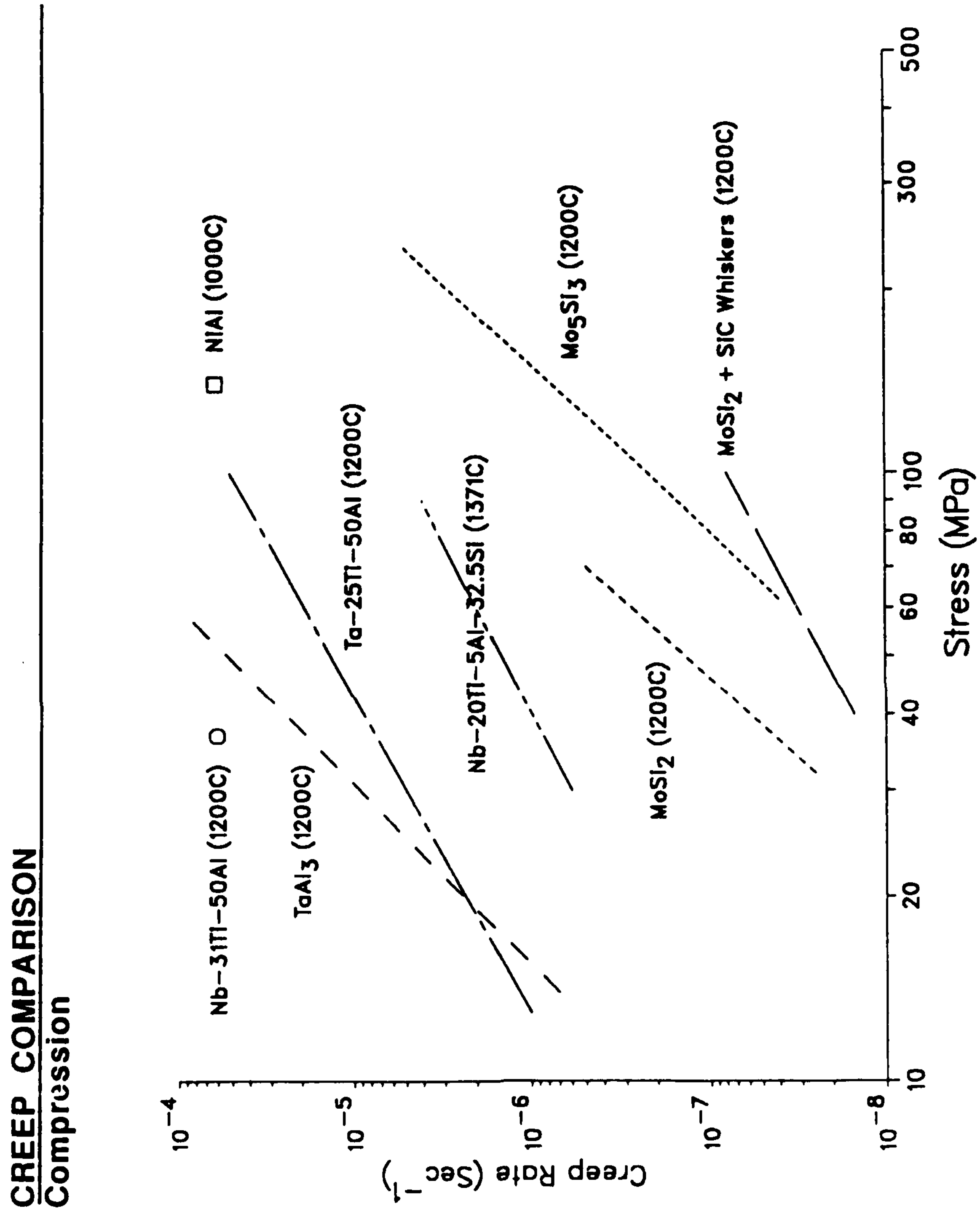
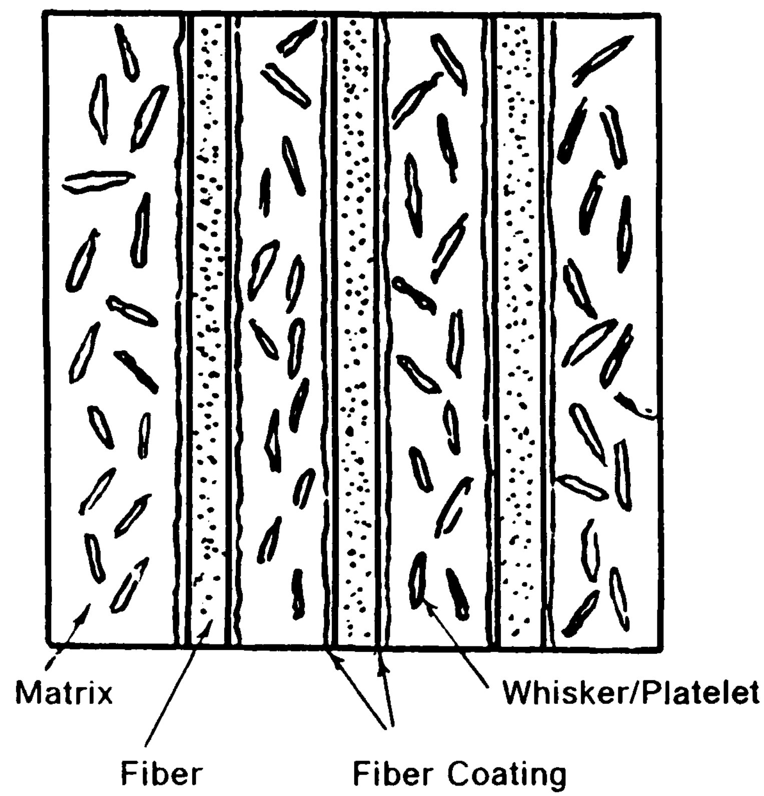

CREEP COMPARISON
Compression
Creep Rate (Sec^-1)
10^-4
10^-5
10^-6
10^-7
10^-8
Stress (MPa)
10
20
40
60
80
100
300
500
Nb-31Ti-50Al (1200C)
NiAl (1000C)
TaAl3 (1200C)
Ta-25Ti-50Al (1200C)
Nb-20Ti-5Al-32.5Si (1371C)
MoSi2 (1200C)
Mo5Si3 (1200C)
MoSi2 + SiC Whiskers (1200C)

Figure 1.

CONCEPT DEFINED FOR STRENGTHENING/TOUGHENING

Applicable for Ta-Ti-Al and $MoSi_2$



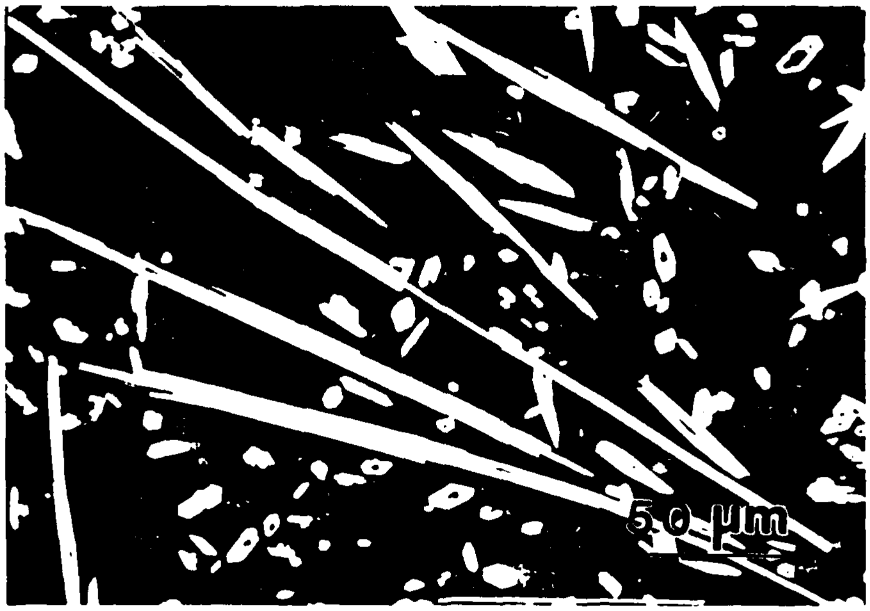
Must Now Address Critical Elements of Compositing

- Whisker/Platelet Dispersion Definition For Matrix Creep Enhancement
  - Could also be used to vary matrix CTE
- Fiber And Fiber Coating Definition
  - CTE match to matrix may be critical
- Processing Definition

Figure 2.

In-Situ Solidified (TaTi)B Boride Needles
in 39Ti-48Al-9Ta-4B Alloy

As Cast



Heat Treated at 1200°C for 100 Hrs.

Figure 3

STRENGTH vs. TEMPERATURE DATA FOR VARIOUS INTERMETALLICS

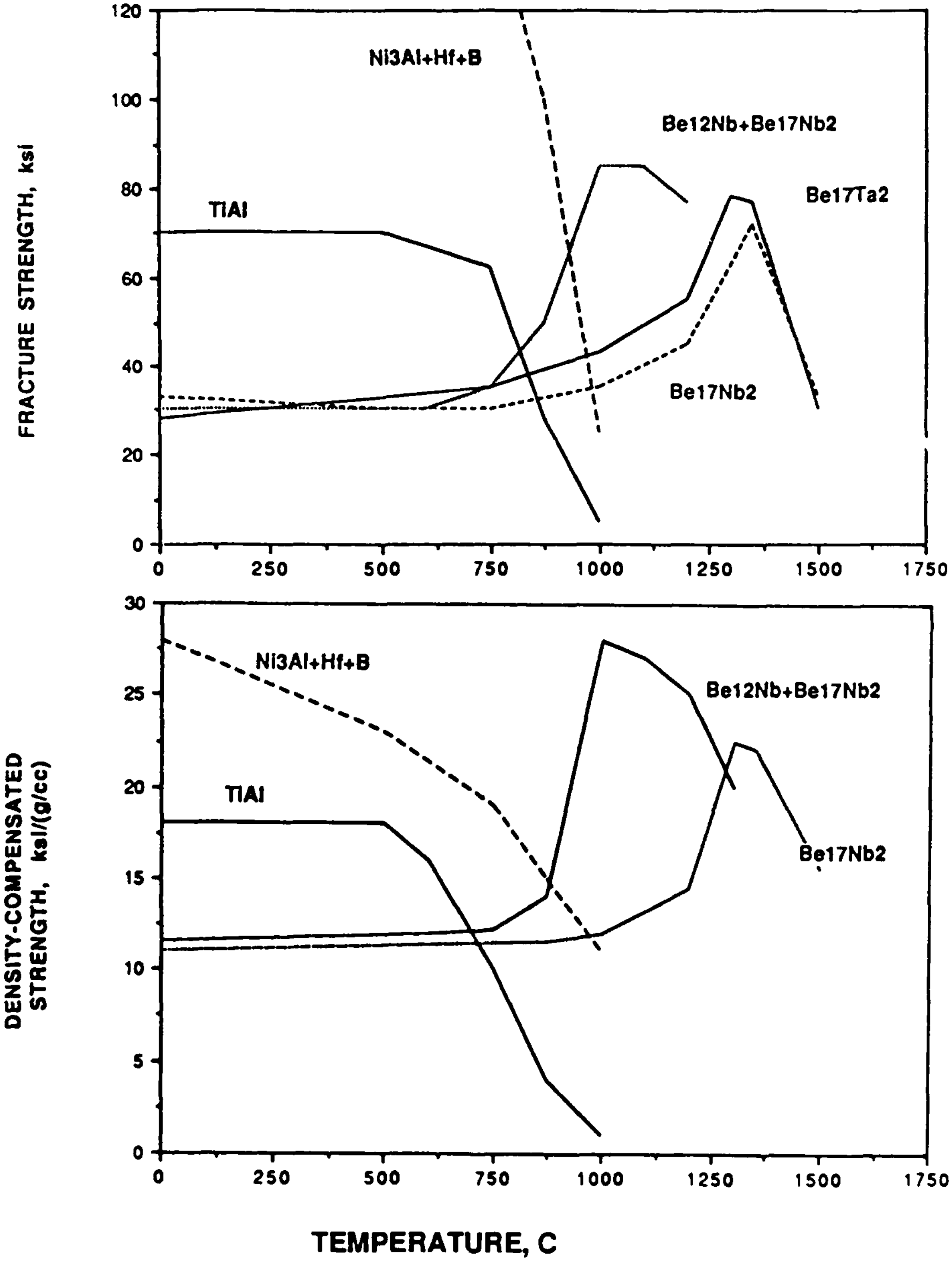


Figure 4.

SUMMARY

1. Candidate Ta-Ti-Al and $MoSi_2$ matrices identified for 1000-1400°C use.

2. Initial efforts underway on beryllides with even higher specific strength at 1000-1200°C.

3. Environmental problems a concern
   - oxidation, water vapor
   - coatings needed with improved mechanical properties

4. Beginning to incorporate alloy design concepts from DARPA/URI program
   - models for microstructure evolution, rapid solidification
   - micromechanics of fiber and coarse particulate reinforcement

Figure 5.

RECOMMENDED ACTION

1. Continued effort on aluminides, silicides and beryllides is warranted because of substantial potential increase in temperature of operation of engines and external structures in high Mach number aircraft.

   - designers accepting low ductility at room temperature

   - promote increased contact between engine/aerospace structure development teams and fundamental work on processing micromechanics/microstructure research.

2. Detailed studies needed beyond screening programs.

   - coating reliability

   - purer base compositions and alloy additions

   - fiber and coarse particulate strengthening/toughening

Figure 6.

NOVEL DEVICES

T. C. McGill, R. Osgood, C. Evans, D. K. Ferry and H. Ehrenreich

EXECUTIVE SUMMARY

OBJECTIVE OF WORKSHOP

Everyone is aware of the great successes in electronics based on Si. However, in recent years devices based on heterojunctions between two dissimilar materials have become common-place and show real promise for becoming the basis for a whole series of novel devices for the future. This workshop was organized to look into some of the more exciting recent developments in this broad area with an eye on DoD systems.

DoD Relevance

The DoD makes use of high-performance, special devices in most of its weapons systems. For example the DoD has major needs for infrared imaging, high-frequency radars, high speed signal processing, and non-volatile memories that can produce reliable storage even in a hostile nuclear environment.

Scientific and Technology Summary

The meeting consisted of six presentations on the broad application of heterojunctions to making novel devices relevant to DoD. DoD has a major effort in infrared imaging. Much of that effort is based on HgCdTe. However, there are concerns as to whether HgCdTe can solve the needs of the DoD. The material is difficult to produce and process to produce uniform arrays of

imagers. Recently a number of new approaches have come to the fore. Results on GaAs/GaAlAs quantum well detectors were reported. While these devices will have individual device performance that is substantially inferior to those produced from HgCdTe, they could be easier to fabricate staring arrays with large number of pixels.

Millimeter wave radar would extend the capabilities of the military in a number of environments. Heterojunction devices are approaching the system requirements for 94 GHz devices. The recent successes with high-electron-mobility transistors (HEMT's), heterojunction bipolar transistors (HBT's) and permeable-base transistors (PBT's) were discussed. The major conclusions are: HEMT's are currently ahead. However, they are limited in their ability to produce high powers at high frequencies. PBT's present fabrication challenges; hence they have not been picked up by any commercial organization. HBT's offer high power, reasonable efficiency and the possibility of attaining the frequency requirements. Research into HBT's could result in the best devices for power amplification in these applications. Standard module approaches may be replaced by arrays of devices that act as a single coherent source with the direction steered by an array of varactors.

The electronics revolution has been produced by taking some standard devices and scaling them to ever smaller dimensions. This strategy for increasing complexity will begin to fail in the early part of the 21st century. New devices that can operate at even smaller scales will be required to continue the revolution. Heterojunction devices could provide the answer. The devices would employ confinement of electrons in one (quantum wells), two (quantum wires) and three (quantum dots) dimensions. The confinement is inherent to the specification of making very small device structures that can be fabricated at

high densities. The characteristic dimensions of the confinement are sub 10nm. Devices based on these structures have been successfully fabricated. Because of some of the difficulties in connecting together such small devices, novel interconnect schemes and architectures are going to be essential to obtaining real applications.

The integration of light emitting and detecting devices with standard VLSI electronics is a very important area of development. Many of the advanced communications systems make use of fiber optic, optical communication systems. Attempts to fabricate III-V semiconductor based optical devices on Si substrates have been partially successful but may not be the near term solution. P. Liao from Bellcore described recent advances in a lift-off procedure for making integrated device chips. In this technology, the opto-electronic devices are fabricated directly in III-V semiconductors. Then the layer containing the opto-electronic device is etched free from the substrate. The thin layer containing the active devices is subsequently attached to the chip containing the more conventional electronics. The major problem is commercialization of this technology since Bellcore does not manufacture.

Silicon is the major electronics technology now and for the foreseeable future. Silicon to date has had the disadvantage that one cannot make heterojunctions and hence exploit some of the novel device concepts that are so important in the III-V arena. In recent years it has become possible to lay down layers of SiGe on Si, hence, giving Si a heterojunction partner. These heterojunctions are strained; that is the lattices do not match. The mismatch in lattice constant is 4% between pure Si and Ge. To exploit these novel heterojunction device concepts in Si, one has to control the strain. Hence, there has been a major emphasis on the fabrication of SiGe/Si heterojunctions under

conditions that would produce epitaxy. Growth temperature is one of the important controlling agents in this area. Efforts in molecular beam epitaxy and chemical vapor deposition have been key in attaining high-quality heterostructures at lower growth temperatures. The applications of these heterostructures might include high speeـ heterojunction bipolar transistors, quantum well IR detectors and tunnel devices, to name a few.

Non-volatile, radiation-hard memories are of major importance to DoD applications. The current systems are very expensive (perhaps as much as $4/bit). The major reason for using such an expensive memory is its non-volatility and radiation hardness. Presentations at this meeting suggested that one might replace this memory with thin film magnetoresistive memory even now. Efforts at Honeywell have demonstrated such memories. Recent discoveries of large magnetoresistance in multi-layered metal structures could be the basis for even higher performance non-volatile memories.

Conclusions

- Heterostructures are going to be very important for DOD applications.
- Quantum-well infrared detectors could offer an alternative to HgCdTe Detectors for some applications despite reduced performance levels.
- Research on devices such as HBT's and advanced and advanced array concepts could yield 94 GHz radar systems.
- New device concepts based on tunneling in heterostructures combined with new architectures show promise for allowing the electronics revolution to continue by shrinking single devices and increasing the complexity of a single chip.
- Lift-off technology permits the combining of optical devices based on III-V's with Si based electronics now. However, it has yet to be

demonstrated that such a delicate process employing thin films of fragile materials can be used in a manufacturing environment.

- SiGe/Si heterojunctions promise to bring about new devices (such as quantum well ir detectors, HBT's well as tunnel structures) that draw on the well developed Si technology.
- Recent advances in magnetoresistive random access memories plus the discoveries of giant magnetoresistance in metal superlattices could yield greatly improved non-volatile magnetic memories.

Recommendations

- DARPA should continue to fund novel applications of heterostructures for devices.
- High-speed devices capable of power gain (HEMT'S, HBT'S) should be developed in conjunction with integrated array technologies.
- Transfer of the GaAs lift-off technology from Bellcore to ' 'S commercial industry should be emphasized to test the manufacturability of this process.
- The effort in novel device concepts and architectures involving lower dimensional structures should be increased given the importance of the payoff.
- SiGe/Si heterojunctions should continue to be an important component of DARPA's program. Emphasis should be placed on non-digital devices such as quantum well detectors.
- Non-volatile memories based on magnetoresistive devices should be evaluated for DoD application. The required basic research should be provided.

AGENDA

WORKSHOP on NOVEL DEVICES

July 18, 1989

Tuesday, July 18, 1989

Introductory Comments (J.D. Murphy, Andy Yang and J. Alexander)

Overview - T.C. McGill (CalTech)

IR Detectors Based on Quantum Wells - S. Lyon (Princeton)

Heterojunction Bipolar Transistors for High Frequency Applications - P. Asbeck (Rockwell)

Trends in Making Small Device Structures - J. Randall (TI)

GaAs Liftoff for Opto-electronics - P. Liao (Bellcore)

Trends in Processing Group IV Semiconductors (MBE, CVD, CBE) - R. J. Hauenstein (HRL)

Nonvolatile Memories Based on Magnetic - G. Prinz (NRL)

GENERAL DISCUSSION

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LIMITATIONS OF PROCESSING FUTURE VLSI CIRCUITS

C. Evans, D. Ferry, B. Gilbert, T. McGill, R. Osgood

EXECUTIVE SUMMARY

Objective of the Workshop: Silicon processing is a rapidly evolving, complex technology which controls the development of future electronics systems and other related semiconductor-based systems. This workshop was organized to determine the key limiting factors in the development of future silicon ultra-large scale integrated circuits (ULSI). The focus of the workshop was the technology beyond that planned by Sematech. Technical, scientific, and business issues were all discussed.

DoD Relevance: Silicon integrated circuits are the central component in most DoD electronic systems for weapons and logistics. Advanced DRAMS and micro-processors provide a reduction in system weight and volume thus enhancing the performance of these systems. In addition, many techniques in silicon processing technology, e.g., lithography can be applied with little modification to other key DoD semiconductor technologies such as IR detectors, optolectronics, and GaAs digital IC's.

Summary of Science and Technology

This two day DARPA workshop was structured to include a particularly wide cross-section of participants including; (a) industry, university, industry

consortium (Sematech), national laboratories and government, and (b) executives, line managers, and basic and applied researchers.

As shown in the agenda, the workshop focused on five areas of ULSI manufacturing: (1) overall trends in manufacturing, (2) lithography, (3) pattern transfer, (4) inter-connects, and (5) packaging.

Many speakers stressed the theme that improvements in current semiconductor electronics manufacturing is limited by the processing complexity. Greater lithographic resolution and more process steps are required for each DRAM generation.

An additional factor limiting the improvement of electronics is the increasing capital cost of succeeding generations of process equipment, viz., the ~$20 M cost of an x-ray synchrotron compared to $3 M for the current generation optical stepper. Equipment sophistication must improve to decrease feature size while maintaining reasonable yields.

The central thrust of advanced silicon processing is to pattern wafers with fine spatial resolution features. Currently, the pattern is established with optical lithography. Spatial resolution down to 0.35μm can be obtained with a 248μm excimer laser source. X-ray lithography, under development, appears to be usable to 0.15 and possibly even 0.1μm, although it may first find use at 0.35 because of its expected higher yields. A possible competitor in the 0.25-0.35μm region is 193-μm excimer laser processing. However, the chief advantage of the laser technique is that it can potentially raise IC yields by eliminating a large number of processing steps. Below 0.1μm, no viable lithographic tools (other than electron beam lithography) are currently under development, although ion projection and vacuum ultraviolet projection (using an FEL or undulator source) offer promise in this region.

Once a pattern has been established, it must be transferred to the substrate generally in the form of surface etching or substrate doping: In this case, ~ $\leq 0.1\mu m$ small-scale lateral resolution appears to be attainable with existing tools; however, there are still very significant fundamental issues of process and materials chemistry and physics. Understanding these issues can often increase the yields of a particular process by an order of magnitude.

Improvements in the device and circuit materials must also be continued for ULSI. Silicide interconnects must be improved via the use of epitaxial materials or high aspect ratio structures, ultimately epitaxial metal structures maybe required. Fundamental changes in circuit architectures may ultimately be required to obviate the need for long interconnect lines.

Finally, the high speed high IO packaging for these chips requires major advances with packaging technology. These include new very fine off-chip wiring schemes and advanced cooling technique, probably based on liquid flow.

Conclusion

(a) The high capital equipment cost, short cycle times and manufacturing complexity put severe pressures on the U.S. being able to remain in advanced silicon manufacture.

(b) Lithography and pattern transfer are key technologies for future VLSI. There is at present no viable lithography tool for resolution less than $0.1\mu m$ (electron beam lithography is still thought to be too slow).

(c) Development times for two key DARPA programs in silicon technology (Sematech and x-ray lithography) are proceeding at too slow a pace to assist the U.S. semiconductor industry.

(d) DARPA procurement time of 1 1/2 years is too slow for DARPA to contribute to near-term technology.

(e) The technology base for advanced silicon VLSI is not being maintained.

Recommendations

A. Initiate a major program in projection, <0.1μm lithography, VUV and ion techniques should be examined.

B. DARPA should not extend its short range manufacturing programs in VLSI because of already significant investment in Sematech and MMFT.

C. The DARPA program in synchrotron sources must be accelerated to match off-shore activities in this area.

AGENDA

LIMITATIONS on FUTURE VLSI

JULY 19/20, 1989

ORGANIZERS: R. Osgood, T.C. McGill, and D. Ferry

Wednesday, July 19 SESSION CHAIR: Barry Gilbert

INTRODUCTION - Dr. Tom McGill, California Institute of Technology

WHERE ARE WE GOING IN VLSI ? - Dr. Gene Meieran, INTEL

0.2mm AND SMALLER: UNIVERSITY PERSPECTIVE - Dr. Fabian Pease, Stanford

ADVANCED SILICON PROCESSING : MANUFACTURING - Dr. Daniel Fleming, IBM

LITHOGRAPHIC CHALLENGES:

STEP AND SCAN TECHNOLOGY - Dr. Charles Karatzas, Perkin Elmer

X-RAY LITHOGRAPHY - Dr. Robert Hill, IBM

SESSION CHAIR: Eric Cross

EXCIMER DIRECT PROCESSING FOR 0.25 m VLSI - Dr. Daniel Ehrlich, MIT, Lincoln Lab.

DESIGN AND TECHNOLOGY CHALLENGES FOR SUBHALFMICRON CMOS AND BIPOLAR TECHNOLOGY - Dr. Tak Ning, IBM/T.J. Watson, Res. Ctr.

LIMITATIONS ON E-BEAM LITHOGRAPHY AND THE PROMISE OF ION BEAM PRINTING - Dr. John Randall, TI

Thursday, July 20 SESSION CHAIR: Mark Wrighton

SEMATECH ADVANCED RESEARCH PLAN - Dr. Ashok Sinha, SEMATECH

PACKAGING FOR ULTRA VLSI - Dr. Fabian Pease, Stanford Univ.

PLASMA PROCESSING AT ULTRAHIGH RESOLUTIONS - Dr. Linda Ephrath, IBM

INTERCONNECTS: SILICIDE/MATERIALS AND ARCHITECTURE - Dr. David Fraiser, INTEL

SESSION CHAIR: Al Tasch

CHALLENGES IN IMPLANTATION APPLICATION FOR DEEP SUBMICRON I. C. - Dr. Thomas Seidel, SEMATECH

ADVANCED TECHNOLOGY PROJECTION VUV LITHOGRAPHY WITH AN FEL SOURCE - Dr. Brian Newman, Los Alamos Laboratory

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LIMITATIONS ON PROCESSING FUTURE VLSI CIRCUITS

PROBLEM: WHAT ARE THE FUNDAMENTAL LIMITS ON PROCESSING SILICON IC CHIPS WITH FEATURE SIZES BELOW 0.25 μm.

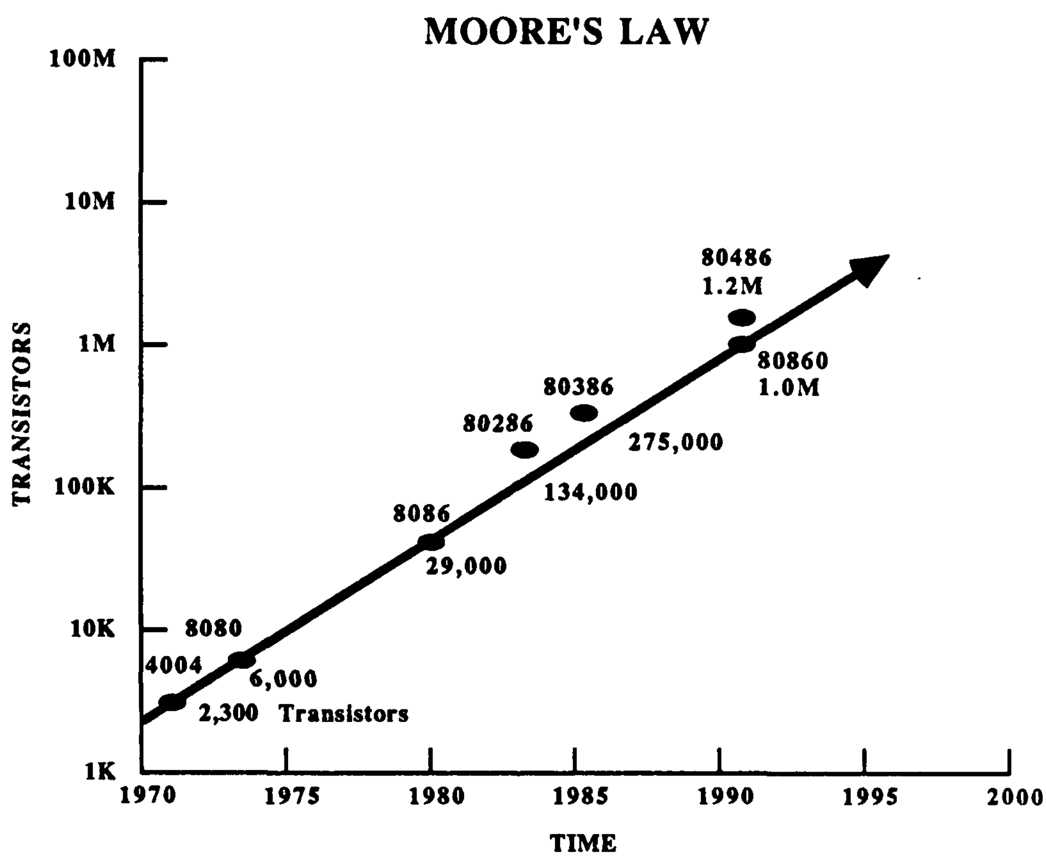
RELEVANCE: ULTRA-HIGH DENSITY SILICON MICRO-CIRCUITS ARE PACING ELEMENTS IN DEVELOPING FUTURE DOD WEAPONS AND LOGISTICS SYSTEMS.

SILICON PROCESSING TECHNOLOGY IS ALSO THE PACESETTER FOR GaAs AND HgCdTe DEVICES AND CIRCUITS.

PROCESSING

- OVERALL PERSPECTIVE
- LITHOGRAPHIC PATTERNING
- PATTERN TRANSFER
- DOPING
- NEW MATERIALS
- ISSUES IN PACKAGING

CHARACTERISTICS OF MODERN SILICON IC FABRICATION



- INCREASING COMPLEXITY
  - NUMBER OF STEPS
  - DESIGN
  - PRECISION ~16M BIT $\approx$ 0.5 μm
- INCREASING COSTS TO WIN
  - R&D
  - CAPITAL COSTS

ADVANCED LITHOGRAPHIES FOR

FOR $\leq 0.1\mu m$

ION PROJECTION

- **INEXPENSIVE AND AVAILABLE SOURCE**
- **MASK DIFFICULT BECAUSE OF LACK OF TRANSPARENT MATERIALS**

VUV

- **REFLECTIVE PROJECTION SYSTEM?**
- **RESOLUTION LIMIT $\sim 0.05\mu m$.**
- **SOURCE NOT YET AVAILABLE.**

Synchrotron X-ray Sources

Ring	Energy (MeV)	λc (Å)	I peak (mA)
• Existing conventional rings (room temperature iron dipoles)			
NSLS VUV (Brookhaven)	750	25	700
BESSY (Berlin)	800	19.4	700
Aladdin (Wisconsin)	800	22.7	150
Photon Factory (Tsukuba)	2500	3.1	150
• Conventional rings under construction			
LUNA (IHI)	800	22	
NTT	800	20	
SORTEC	1000	15.5	
CAMD (LSU)	1200	9.5	
• Superconducting dipole rings under construction			
SUPER ALIS (NTT)	600	17.3	
COSY (Berlin)	590	12	
NIJI III	620	11.7	
AURORA (Sumitomo)	650	10	
SXLS (BNL)	700	10	
HELIOS (Oxford)	700	8.5	200 (plan)

RESEARCH ISSUES

- NEW SENSOR TECHNIQUES
- ADVANCED INTERCONNECT MATERIALS AND DESIGNS
- INTERFACIAL CHEMISTRY
- SIMPLIFIED PROCESSING
- NEW ARCHITECTURES

SUMMARY

- INCREASINGLY HIGH CAPITAL EQUIPMENT (\$1M), SHORT CYCLE TIMES (1 1/2 - 3 YRS), AND COMPLEXITY CHARACTERIZE MODERN SEMICONDUCTOR FABRICATION LINES.
- LITHOGRAPHY AND PATTERN TRANSFER ARE KEY TECHNOLOGIES FOR FUTURE VLSI; THERE IS AT PRESENT NO OBVIOUS VIABLE LITHOGRAPHY TOOL FOR RESOLUTION AT OR BELOW 0.1 μm.
- DEVELOPMENT TIMES FOR TWO KEY DARPA PROGRAMS, SEMATECH AND X-RAY LITHOGRAPHY PROGRAM, ARE PROCEEDING AT TOO SLOW A PACE TO BE EFFECTIVE, *VIS A VIS*, OFF-SHORE COMPETITION.
- DARPA PROCUREMENT TIME OF 1 1/2 YEARS IS TOO SLOW FOR CONTRIBUTIONS TO NEAR-TERM TECHNOLOGY, INHIBITING FOR MEDIUM-TERM TECHNOLOGY.
- THE TECHNOLOGY BASE IN ADVANCED SILICON IC'S IS NOT BEING MAINTAINED.

RECOMMENDATIONS

- DARPA SHOULD NOT EXPAND ITS NEAR TERM MANUFACTURING PROGRAMS IN SILICON VLSI BECAUSE OF ALREADY SIGNIFICANT INVESTMENT IN SEMATECH AND MMST.
- THE DARPA PROGRAM IN X-RAY SYNCHROTRON SOURCES MUST BE ACCELERATED TO MATCH OFFSHORE ACTIVITIES IN THIS AREA.
- INITIATE A MAJOR PROGRAM IN PROJECTION TECHNOLOGY FOR $< 0.1 \mu m$ FEATURE SIZE.

  a) LITHOGRAPHIC SYSTEMS - VACUUM ULTRAVIOLET
  ION PROJECTION

  b) PATTERN TRANSFER

COMMENTS ON "ADVANCED VLSI PROCESSING"

C. A. Evans, D. Ferry, T. C. McGill, R. Osgood

INTRODUCTION

This report summarizes several key insights learned from the workshop. The intent is to supplement several briefer, but important, statements made in the executive summary.

The intent of the workshop was to obtain a clear, overall picture of the limiting technology in processing very advanced silicon VLSI. In the workshops, "advanced" was loosely defined as IC's with linewidths less than 0.25 mm.

PROCESSING COMPLEXITY AND THE COST OF BEING IN BUSINESS

Several speakers, from corporate Vice President (G. Meieran) to university professors emphasized the impact that processing complexity was having on IC manufacture. The complexity comes directly from increasing die and wafer sizes, and the decreasing dimensional scale on the patterned chip. The first and third of these trends increase the number of components per chip, Fig. 1. The second trend greatly increases the care and difficulty of establishing process tools. While these changes reduce the overall cost of a silicon IC, they simultaneously raise the cost of being a participant in manufacturing silicon IC's.

Increasing complexity raises the cost in many areas of semiconductor manufacture. For example, in his summary of the emerging technology of VLSI, Pease illustrated the escalating costs by giving the case for the basic tool for

photolithography. In 1976 basic mask aligner for producing μm features cost \$140K, by 1988, the cost of the most advanced Perkin-Elmer tool had risen to \$3M. In the near future, X-ray lithography is expected to play a key role and the cost of the storage ring required will be \$15-20M. These costs in capital range across the board from cluster etching tools to advanced epitaxial systems. The costs are such that only the largest companies can remain in IC manufacturing.

Complexity also appears in the number of processing steps. The use of complex materials, such as silicides, or the need for absolute planarity during photolithography, all require the adoption of more masking levels and thus put stress on the overall yield for manufacture. To the same extent this trend can be reduced by the adoption of simplifying processing techniques such as the 193nm, excimer laser chemical processing described by D. Ehrlich at Lincoln Laboratory, Fig. 2. Another approach to the problem is to improve the human engineering of each processing module, and to improve the work force quality to the point where yield is increased by closer control of the fabrication parameters of each step, Fig. 3. Again, the resources for this later approach are demanded in terms of better tool design (higher costs) and a better trained workforce; all require greater costs to stay in manufacturing.

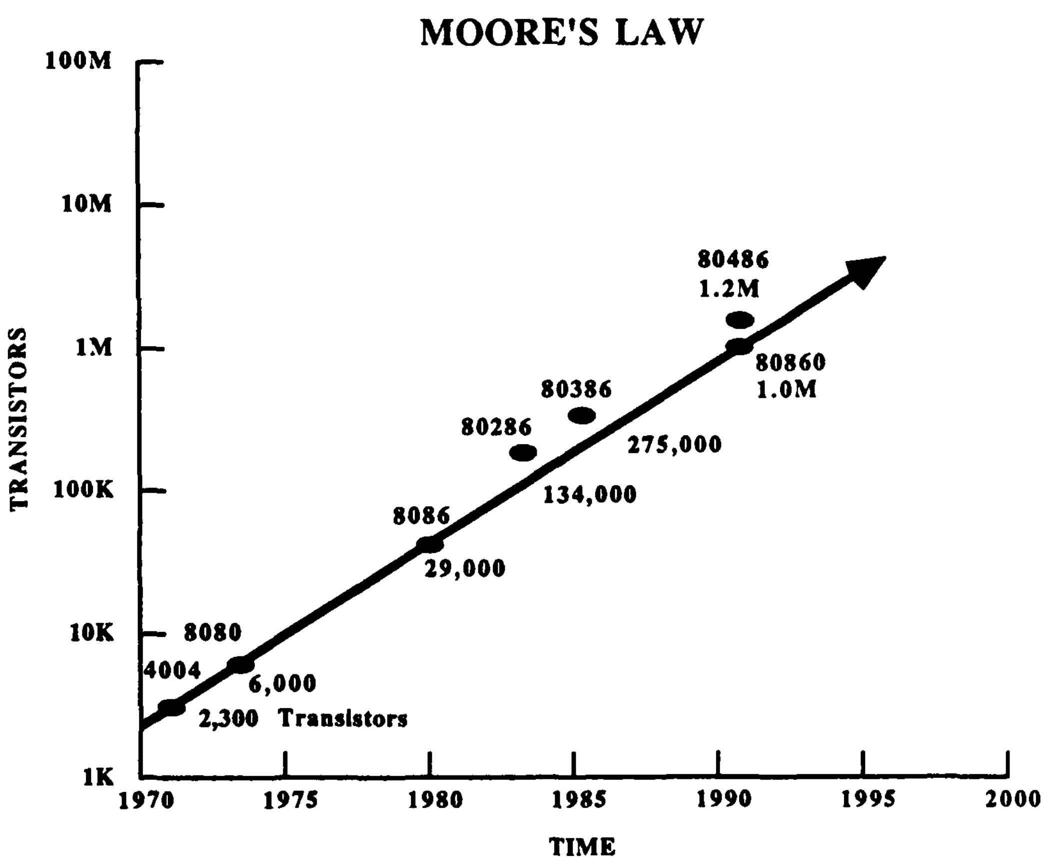
TECHNOLOGY BASE FOR SILICON INTEGRATED CIRCUITS

The increasing complexity in silicon technology requires a significant base of basic and applied materials research to realize each new generation of IC. As shown in Fig. 4, the materials needs generally fall in the classes of new materials, e.g., GaAs on Si (or Si:Ge on Si), and in advanced processing, e.g., ultrafine lithography.

Because of the high competitive nature of Si electronics and the quarterly reporting, demands of American corporations, the necessary research for these

advances can not occur except in the very largest corporations. The result is that the technical base, which was the sine qua non of American leadership in electronics, is currently eroding rapidly.

A good example is X-ray lithography, which has need for slower resists (in order to increase contrast) and more intense sources. Hence, there is a need for more work on viable storage rings sources.



FACTORY AUTOMATION

Figure 1.

COLLAPSE OF THE LITHOGRAPHIC CYCLE

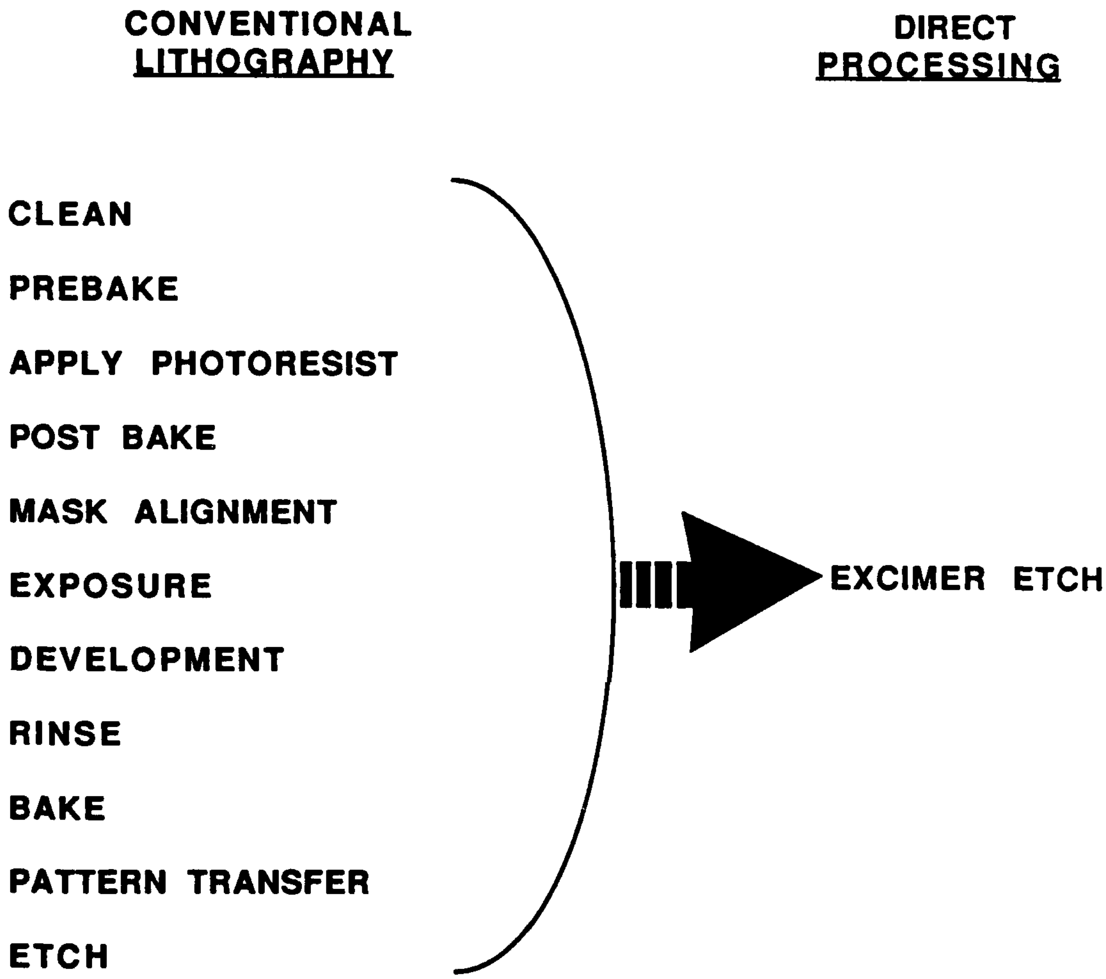


Figure 2.

PEOPLE

- ELIMINATE PEOPLE HANDLING WAFERS
  - ROBOTICS
  - CONTROL WAFER ENVIRONMENT
- PEOPLE OPERATE, DIAGNOSIS, MAINTAIN
- ADVANCES IN SKILLS REQUIRED
  - PROCESS OPERATOR → TECHNICIAN
  - BASIC SKILLS IN: TECHNICAL MATH
    CHEMISTRY
    PHYSICS
    MATERIALS
    ELECTRONICS
    PROGRAMMING

Figure 3.

Process

High complexity demands smaller feature sizes

Multi-level non-Al metallization

Dry etching

Electron beam and X-ray lithography

Mixed processes (Si/GaAs)

Mixed technologies (analog and digital)

Figure 4.

ADVANCED PACKAGING FOR DIGITAL SILICON AND GaAs

R. Osgood, B. Gilbert, J. Economy, L. Cross

The workshop on Future Limitations on VLSI, indicated that there is a critical need to develop a broadly based program in packaging science and technology. This program is necessary to address the rapidly developing gap between microchip capabilities and the ability to interface this capability with the electronic system via the package. In fact, in the one area of advanced high speed multichip packaging, this need is sufficiently critical that a pilot line capability is needed. Specific needs in advanced materials include 1) lithographically optically processible insulating layers with very low dielectric constant, 2) metal circuitry with much higher electrical conductivity, 3) low stress interconnects which minimize critical concerns with reliability, 4) improved processes for removing heat from the chip and 5) new kinds of easily processed encapsulants which provide long term protection against the environment.

In this memorandum we would like to first discuss the current critical situation with regard to the packaging requirements for advanced silicon and GaAs. We will then present the need for an advanced package pilot line; finally we will stress the need for a continuing growth in the technology base. This discussion will emphasize novel structures, high speed considerations, materials issues and processing techniques. We point out that the MRC meetings in the last two successive years have identified and discussed many of these same issues; many useful details are given in the reports from these meetings

Within the last several years the increases in pin count and speed in silicon ECL circuits and ultrahigh speed GaAs digital circuits have made major

new demands in advanced electronic packaging technology. In particular, high speed performance requires packages with low dielectric permittivity materials such as are found in organic insulators, e.g., polymide, and high-conductivity ground planes and conductors. The cross talk and frequency response of such structures makes electromagnetic modeling essential. Making such multilayer structures out of materials non-traditional to the electronics communities has raised many questions on new fabrication techniques, adhesion and interfacial stability. The need for high interconnect density and cooling for silicon circuitry, and particularly for GaAs circuitry, requires novel design for fine line interconnects and conductors in the package.

The multichip package (MCP) is an important near term answer to the packaging problem for both GaAs and Si. In this case anywhere from several chips, to as many as ~100, are mounted in a large multilayered package structure. The dense interconnects in this structure are designed so as to be nearly an extension of those on the chip. In the past decade multi-layer ceramics (MLC) with 33 levels of circuitry were developed by IBM for the large main frame computer of the 1980's. The MLC, which consists of silk screened molybdenum conducting lines and an aluminum oxide dielectric, however, is not compatible with the high speed chips currently under development. For the future, fine line circuitry (optically or lithographically processed) will be required along with insulating layers approaching dielectric constants of 2.0. In addition, far more sophisticated concepts for laminating multilayer structures with features 1/10th the dimension of current packages must be explored. These range from the use of photoimageable insulating layers to stacking and densifying lithographically processed fine line layers to achieve the desired properties.

MCP Pilot Plant

As discussed in the introduction, the combination of high wiring density and high clock rates in (the state of the art) GaAs and Si ECL circuits require multichip packaging. Although several US firms, i.e., GE, Honeywell, and Boeing have development programs to build such packaging, principally under DoD sponsorship, no US firm currently markets these packages commercially. As a result, many of the high speed GaAs IC's made by DARPA cannot be used in the systems. Thus there is a critical need for an advanced MCP pilot plant which permits a scaled-up evaluation of new concepts for designing and evaluating the wide number of approaches currently under consideration. These include:

1. design of MCPs consisting of many chips interconnected to only a module or a board

2. evaluation of new kinds of high modulus rod-like polymers which act as both substrate and insulating layer

3. use of new approaches for registering and laminating of many layers in a parallel manner

4. design of alternative processes for heat removal as well as improved encapsulation

5. process simplification through use of new kinds of photoimageable insulating layers are new techniques to effect photoimaging

6. design of systems intended to function at liquid nitrogen temperatures to better exploit improved electrical conductivity of metals.

Supporting Technology

Unlike much of the semiconductor device and IC technology, the packaging expertise in the US has largely grown without a strong supporting tech-base program. As long as packaging remained at the state of the art of simple single chip alumina carriers and dual in-line packages (DIP) this approach sufficed. Unfortunately, packaging electronics requirements are now as demanding as those for the IC's themselves. As a result, it is not surprising that the previously *ad hoc* approach to package development is no longer valid. Major and very sophisticated scientific issues must be solved if more advanced packaging is to be developed.

Processing Techniques

The preparation of semiconductors and other materials for IC applications has in many ways paced the development of new materials processing technologies in general. The very stringent requirements for IC performance demanded and yielded new methods of materials growth, etching, annealing, etc. In a similar fashion the emerging requirements for electronic packaging will necessitate new approaches to the processing and fabrication of the packaging materials. This point is clearly illustrated by the fact that four of the multichip packaging efforts in the United States, i.e., GE, Boeing, IBM, and n-Chip had to have used novel laser processing techniques in developing their packages.

The complex structure and unusual material combinations in advanced packaging impose important requirements on processing techniques. Processing operations such as etching and metal growth must be done at low temperatures to prevent degradation of the polymer dielectric layers and in particular the metallization itself. The high cost of many packages, such as the

IBM MLC package, means that techniques for repair and incorporating engineering changes must be developed. The lack of absolute planarity on the package surface means that nontraditional methods must be used for patterning. (See section on Novel Structures.)

Materials Issues

Many of the materials challenges for developing high-performance packages stem from the fact that the materials to be used are completely different from those in previous IC technology, by virtue of the strongest requirements of the demanding electrical and mechanical requirements.

I. New low dielectric permittivity materials for packaging:

The research goal in this area is to obtain dielectric insulators with permittivities less than 2. These dielectrics are necessary to minimize crosstalk for closely packed interconnects. The use of conventional ceramics such as the alumina in the IBM MCP is completely ruled out for signal plane structures by the need for very low dielectric constants.

Two approaches are feasible for advanced packaging. The first is the use of polymeric dielectric layers such as polyimides. In fact, the current MCP's being developed for the DoD use polyimide dielectrics. Nonetheless, much work remains to be done before these organic dielectrics can be regarded as satisfactory. Polyimides have a tendency to be sensitive to environmental factors such as water vapor and thermal stress. Polymers as a family are generally not radiation hard and have inadequate thermal stability. Clear cut goals for design of improved polymeric insulating layers include development of systems which have dielectric constants approaching 2.0, are photoimageable, are stable thermally and structurally at 400°C, planarize over topography, are

inert to moisture, display a thermal expansion coefficient similar to silicon or GaAs and will form a strong adhesive bond to previously deposited layers. A number of polymers have been developed which meet many of these requirements. However, the critical task facing polymer materials scientists is the goal to design systems which meet all these needs.

The second class of dielectrics uses porous ceramics or polymers to achieve ultralow dielectric constant K>1. Porous ceramics have been used to make simple single-layer metal dielectric structures. The primary research issues in the area are to determine optimum pore size, to develop reliable foaming techniques for inorganic materials, and to develop methods of laminating these structures to yield packages with the necessary structural integrity.

II. Interconnects:

In his talk at this year's VLSI workshop, F. Pease pointed out that the fundamental limits to the density of interconnects in an MCP is set by the resistivity of the conductor. As a result, methods for improving conductivity are the key to improving package effectiveness. The most straightforward approach is to use higher conductivity metal lines, novel line geometries or stacked structures. A second avenue is to operate at liquid nitrogen temperatures to greatly reduce the resistance of metal lines; the use of high T_c superconductors may also be feasible.

Another serious problem concerning interconnect technology is the fatigue associated with the mismatch in the coefficient of thermal expansion (CTE) between the chip and substrate. This problem is undoubtedly the single greatest contribution to loss in reliability in packages.

III. Interfacial chemistry:

The sharply dissimilar materials used in packaging, e.g., metal on polymer on ceramics, place new demands on understanding interfacial chemistry. Mechanical and thermal stresses strain these interfaces (see 1988 MRC report). Chemical stability can also be a problem -->. In particular, adhesion of metals to polymers can be poor without ion bombardment or some other technique for modification of the surface chemistry or topology.

Unfortunately, such processes frequently change the chemical composition of the polymer, making the interface far more sensitive to attack by moisture. Again, design of polymers which better match the CTE of the metal would go a long way toward minimizing this problem.

High Speed Considerations

Until very recently, modeling of the frequency response of package interconnects has been based on the use of simple, lumped-circuit calculations. At GHz clock rates, which are being achieved in Ga:As ICs, this approach is inadequate, and careful electromagnetic modeling must be adopted. Realizing that even the most ambitious theoretical modeling techniques will likely not be adequate for optimizing package design, experimental techniques must be developed for probing electrical signals in actual high speed packages or closely related model structures. Again, techniques recently developed for measuring the electrical response in high speed IC's may have applicability for packages.

Novel Structures

An important point made in this year's VLSI workshop was that a driving force for even more complex VLSI is the high cost in dollars and power of off-chip interconnects. Another way to achieve this same function is to use advanced packages with near VLSI-like conductors. In this area, new approaches for novel structures can yield major advances in packaging capabilities.

There are several examples of problem solving by radically new package design. The first example is concerned with the fact that MCP's for silicon ECL are limited to a large extent by the ability to cool the package. IBM's ceramic MCP, for instance, used an elaborate piston approach to solve the problem. However, a far simpler and more effective approach used direct water cooling of a silicon wafer substrate on which silicon chips are mounted. This approach enables a factor of ~1000 improvement in the maximum allowable chip heat load. The net result is that the ECL circuits can be run faster.

A second area of package structure improvement has been in approaches to making chip interconnects. Multiple, high density connections are the key to making the best use of the package capabilities. The basic problem with making these interconnects is in connecting to the chip from the package with the necessary fine line resolution. The non-planar topography at the chip package junction prevents joining by lithography. Two novel approaches have been recently used to solve this problem. One uses laser writing to "write up" a gold line connecting from an interconnect on the substrate to a chip, another uses an etched metal covered SiO_2 cantilever structure to make the necessary bond.

Both of the above examples show that completely new approaches can be formed to solve very fundamental structure problems in packaging.

Summary

The VLSI workshop reiterated earlier studies which have highlighted the "bottleneck" which is developing in adequate multichip packages for the new ultra high speed Ga:As ICs which are the product of DARPA sponsored programs. It is suggested that a pilot line capability be set up to act as the test bed for advanced multichip package designs, but that there is also urgent need for expanded research both on the electromagnetic designs and on the diverse materials systems which will be required in these vital packaging systems.

INSULATORS

DESIGN CRITERIA FOR ADVANCED INSULATORS

- Stability to 400°C
- Elongation > 10%
- Tg > 400°C
- Planarizable
- Low moisture uptake
- Dielectric Constant <2.7
- Solvent Resistant
- Photosensitive
- Low T.E.C.

PROBLEMS WITH ORGANIC INSULATORS

- Poor Adhesion
- Corrosion at Metal Interfaces
- Nature of Oxidized Surfaces
- High Transport of H2O
- Anisotropic swelling

RESISTS

DESIGN CRITERIA FOR ADVANCED RESISTS

- Ultra Sensitivity < 5m J/cm2
- Thermal Stability > 120°C
- Tg > 100°C
- Isotropic Casting
- Stable to dry etchant

PROBLEMS IN LITHOGRAPHY

- Resist Aging
- Adhesion loss (dvpt)
- Redeposition of resist (dvpt)
- Non-uniform profiles

SENSORS IN SEMICONDUCTOR DEVICE PROCESSING

C. Evans, R. Osgood, G. Whitesides, J. Economy

EXECUTIVE SUMMARY

The manufacture of advanced semiconductor devices requires increasingly complex processes, very expensive equipment and an increasing number of processing steps. Each processing step has the potential to advance or inhibit throughput and device yields. The question addressed by this workshop: Can the inclusion of analytical probes and sensory in the manufacturing process: (1) Improve the overall manufacturing of semiconductors? (2) enable new manufacturing processes or devices? or (3) enhance manufacturing yields? The insertion of existing or the development of new probes would either be used to monitor the process to maintain the processing window or be used in a feedback loop so as to control a process when the processing window is tight.

The relevance to DoD is that improved semiconductor processing technology and yields will enable improved manufacture of silicon and gallium arsenide-based digital integrated circuits and electro-optics.

The workshop was divided into two sections:

1. First were presentations on the status of in situ processing in the silicon and gallium arsenide communities as represented by IBM, Gigabit Logic and SEMATECH.

2. This section was followed by some specific discussions on probes and sensors which had been or were proposed for insertion into the

semiconductor processing environment. These presentations focussed on optical methods due to their lack of intrusion into the process itself.

A summary of the presentations includes:

1. There exist certain sensors or probes which can be readily inserted in certain processes and provide meaningful results. These include residual gas analyzers and optical emission spectrometry from plasma based processes.

2. There are certain processing steps which need the development of better probes or sensors. These include end point detection for plasma based/reactive ion etch, CVD thin film deposition and surface contamination.

3. The inclusion of process sensors and probes can be highly leveraged since modern process equipment is very expensive (1-3M$).

4. The real time process control program at SEMATECH looks promising. As a pilot study, they will shift process module control from machine parameters to plasma parameters using off-the-shelf diagnostic tools and response function algorithms.

5. IBM has demonstrated the critical importance of sensors in actual production environment. The applications include the detection of plasma contamination and improved end-point detection using optical emission spectroscopy. The most significant result was the detection of plasma generated particles using light scattering techniques and the prediction of the on-set of particle generation using laser induced fluorescence.

6. There is a wide difference in the receptivity to in-line process monitoring. The process development engineers in the U.S. and Japan want the inclusion of sensors while the manufacturing floor managers (U.S. and Japan) want no intrusion which might alter or contaminate the process. The

U.S. GaAs manufacturers do want improved monitoring. U.S. equipment manufacturers are not participating.

Our recommendations are:

1. The near-term sensor needs of DARPA should be addressed by DARPA/SEMATECH Program.
2. A focussed DARPA effort should:

a. Address one or two specific processing steps in GaAs technology.

b. Processing step should be chosen for relevance to Si and GaAs manufacturing.

c. Program should be jointly pursued by GaAs manufacturer, the "researcher" with the sensor concept or technology and a US manufacturer of the process equipment.

INTRODUCTION

The manufacture of advanced semiconductor devices requires increasingly complex processes as well as an increasingly larger number of processing steps has the opportunity to improve yields or to inhibit turnaround time and/or device yields. There exists a large number of analytical instruments and characterization concepts which are presently in the research and development laboratory or available outside the fabrication facility. The question is, can these probes or sensors be advanced and interfaced into the manufacturing process so as to (1) improve the overall manufacturing of semiconductors, (2) enable new manufacturing processes or devices or (3) enhance manufacturing yields? The insertion of existing or the development of new probes would either be used to monitor the process to be sure that the processing window is being maintained or could be used in a feedback loop so as to control a process when the processing window is tight.

The relevance to DoD is that improved semiconductor processing technology and yields will enable improved manufacture of silicon and gallium arsenide-based digital integrated circuits and electro-optics.

The workshop was divided into two sections:

1. First were presentations on the status of in situ processing in the silicon and gallium arsenide communities as represented by IBM, Gigabit Logic and SEMATECH.
2. This was followed by some specific discussions on probes and sensors which had been or were proposed for insertion into the semiconductor processing environment. These presentations tended to focus on optical methods due to their lack of intrusion into the process itself.

There exists a variety of laboratory scale probes and sensors which are amenable to the processing techniques used in the semiconductor industry. In addition, there is a reasonable understanding of what information can be provided concerning the process. These include parameters such as the purity of the environment as well as species to be monitored for end point detection. Interfacing or insertion of these probes remains to be the specific area. Based on the presenters, there is a critical need for specific probes to be developed for certain processing areas. These include but are not limited to end point detection in dielectric layer removal in gallium arsenide technology. Gigabit Logic informed us that over-etching or under-etching of a silicon dioxide layer or the gallium arsenide surface can change the pinch off voltage by one millivolt per three Angstroms or material removed. Unfortunately, they do not have the end point detector that they wish. Other areas of specific focus or need as stated by both the IBM and the Gigabit speakers were a concern over surface contamination at each semiconductor processing step. These inadvertent contamination of the surface by elemental impurities, hydrocarbon contamination or compositionally non-specific particles.

One area that was seen as critically in need of in-process monitoring was CVD growth of thin films. There seems to be very little activity in this area. The only real information that we heard was from Emcore which manufactures OMVPE deposition systems for gallium arsenide. They are developing photo-reflectance techniques in order to probe the surface electronic structure of the growing film.

Throughout all the discussions of semiconductor processing in this workshop as well as others, the high capital cost for each processing step, i.e., piece of equipment, was emphasized. With this very high capital cost, the cost

of developing and inserting a sensor or probe takes on a rather small cost compared to the capital cost and can yield very high leverage by increasing throughput or yield for a given expensive processing piece of equipment.

Although there was reluctance on the part of the silicon semiconductor equipment manufacturers and the fabrication facility manufacturers to allow sensors or probes into the equipment, we found that the gallium arsenide community was begging for more assistance and control in their processes. This is probably a cultural event since many of the manufacturing managers in the gallium arsenide industry were quite recently in the research and development lab and can remember the value of materials characterization.

The presentation by SEMATECH was very heartening in that we feel that their in-house sensor program shows a great deal of promise for advancing the process monitoring in the near term. At the present time, they are collecting a variety of existing probes and sensors from commercial sources to be integrated into existing cluster tooling for particular semiconductor processing steps. Once these are integrated, the relationship between diagnostic data and system performance will be established and a feedback loop closed.

The one success story for the insertion of sensors and probes into the manufacturing environment was found at IBM. After sustaining significant setbacks as a result of unknown processes and lack of control, the manufacturing environment has opened to the analyst and has permitted two types of process monitoring to be developed. In one case, they are working toward inserting a particular measuring device, light scattering, for the examination of particles produced during reactive ion etching. This observation of particle formation has been studied as to other plasma parameters. Using Laser Induced Fluorescence, they have found that particle formation is

preceded by a large concentration of negative ions. In addition, a crash cart approach has been developed such that when a problem is encountered in the fab, specialists bring equipment, housed in the fab, to the site of the disaster and try to debug the process. Thus, IBM has demonstrated the critical importance of sensors in the actual production environment.

We were very disheartened by the lack of participation in this process by U.S. process equipment manufacturers. Not only did a particular manufacturer not wish to attend the workshop at this time, but it is our understanding they have also withdrawn their support from SEMATECH.

The attitudes in Japan are perceived to be similar and different from those in the United States. The process development community very much wants in situ monitors and sensors for helping to understand, control and develop particular processes. The process equipment manufacturers in Japan seem to be more interested in the inclusion of sensors than in the U.S. The attitudes of the manufacturing managers in Japan seem to be similar to that in the U.S. in that they do not wish anybody intruding into the process and potentially changing or contaminating it.

Given the above success stories and cultural problems, we feel that DARPA should undertake a carefully focused activity in this area, utilizing the enthusiasm of some in order to overcome and redirect the reluctance of others. Recommendations include:

1. The near-term sensor needs of DARPA should be addressed by the DARPA/SEMATECH program. The in-house sensor program at SEMATECH seems to be well thought out and headed in the right direction. But as is always the case, it is a few people working in a highly important area and they could significantly benefit by interaction with others so as to prevent any narrow or parochial attitudes being developed.

2. DARPA should initiate a focused program which would address a critical processing step in gallium arsenide integrated circuit fabrication. This would capitalize on the enthusiasm of this community and should be a joint effort involving a specific step in the gallium arsenide fab, a researcher with the probe or probes of choice and an equipment manufacturer who will be involved in the interfacing of the solution to the problem. This should be a three-way contract and agreement with very carefully controlled goals.
3. An adjunct to the above recommendation is that this problem area or processing step should be chosen for its relevance to both silicon and gallium arsenide processing steps. Not only would this then advance a militarily critical device, i.e., gallium arsenide integrated circuits, but could be used as a role model in order to guide others in commodity and consumer devices as the the value of sensors in the processing environment.

SEMICONDUCTOR PROCESSING AND SENSORS

July 21, 1989

Friday, July 21

Status and Future Needs

Silicon - John Deines, IBM

GaAs - Bryant Welch & Mark Wilson, GBL

A (not the) Perspective from Japan - Drew Evans, MRC/CE&A

Terry Turner, Sematech

Some Ideas for Sensors

Optical Probes - Gary Selwyn, IBM

Proton Tomography - Art Portau, Sandia Livermore

Process Diagnostics in MOCVD - Peter Norris,Emcore, Inc.

Materials Issues - Jim Economy, U of Ill./MRC

Summary - R. Osgood

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ADVANCED ACOUSTIC SENSORS
US NAVY NEEDS

L. E. Cross

(1) LARGE HULLMOUNTED ARRAYS
Vital Parts
(a) Sensor Plane

(b) Outer Decoupler. (Flow noise decoupler)

(c) Inner Decoupler (Platform noise decoupler)

SENSOR PLANE
Piezoelectric Alternatives

- PVF2 or modified PVF2 polymer
- 0:3 Lead titanate: neoprene rubber
- 1:3 Lead titanate zirconate: epoxy polymer

1.1 • PVF2 and Derivatives
Realizable but very expensive. Needs thick film:

-EMI voided film now out of business

-Pennwalt makes by lamination of thinner films
Uniformity, reproducibility and aging of Pennwalt films unknown.

Why is the PVF2 Sensor expensive?

(1) High transverse coupling through d_{31} needs stiff backing and careful design to avoid transverse mode resonances.

(2) Low dielectric permittivity - needs expensive high impedance low noise amplifiers which must be mounted very close to the sensor.

Questions regarding the PVF2 research program.

(1) Will the plasticized PVF2's which show higher permittivity (ε_{33} - >30) also have higher d_h so that the advantageous $g_h = d_h/\varepsilon_{33}$ of the PVF2 is retained?

(2) Can the field assisted crystallization be applied to thick section PVF2, or can thin sections of field crystallized PVF2 be bonded by the Pennwalt method to form thick sheet?

(3) What will the uniformity and reproducibility be, and who will make large sheets of the modified polymers?

1.2 • <u>0:3 Lead Titanate:</u> neoprene rubber or polyurethane composite

Realizable: Less expensive than PVF2.

Advantages:
Higher dielectric permittivity ε~50 - lower cost preamplifiers.

Lower transverse coupling - simple design - no need for lateral stiffening.

Very flat frequency response to $50KH_z$.

No pressure dependence to 7MPa

Problems:

Aging behaviors unknown.

Who will produce the material.

Due to uncertainty over Navy needs several major potential suppliers have lost interest including Celanese, Cyanamide, Raychem, Honeywell.

Westinghouse material not yet of the quality and reproducibility of NGK 0:3 composite.

1.3 • <u>1:3 Lead Zirconate Titanate</u>: Epoxy Composite

Unrealizable using present technology

Need: Economic method to assemble large areas of 1:3 composite.

Present dice and fill techniques from bulk ceramic uneconomic for large area.

Possible Alternatives:

- Super loom as at FMI - automatic post placement already used in three dimensional woven composites.

- Co-extrusion of PZT and thermoset polymer; needs a source of continuous PZT fiber.

Potential Advantages of 1:3 Composite.

(1) Very large $d_h g_h$ product coupled with very high values of piezoelectric thickness coupling k_t.
(2) Can be used in both transmit and receive modes.
(3) Very high permittivity ε_{33} - simple low cost amplifiers.
(4) Low transverse coupling - simple design.
(5) May be an essential component for an active (smart) composite inner decoupler.

2 • <u>Outer Decoupler</u>

Realizable using current technology.
High special frequency of flow noise integrated out by large area hydrophone - possible to use simple passive damping.

3 • <u>Inner Decoupler</u>
Not realizable with any presently available technology.
Broad spatial and temporal frequency ranges of platform noise cannot be extracted with realizable passive systems.

Probably will require smart composite for active noise cancellation.
High k_t of 1:3 composite will probably make this material an essential component in any active damping system.

2. Towed Array
Sensor length 40 cm.

(1) Conventional system PZT capped cylinders
4/sensor length
Problems - expensive: much manual assembly
Advantage - excellent sensitivity
low sensitivity to extraneous noise sources

(2) Lead Titanate - solid block sensors
67/ sensor length
Problems - complex system
Advantage - high sensitivity
Could be replaced by simple 3:0 composite

(3) 0:3 Lead Titanate : Polyurethane composite
1 element / sensor length
Problem - unknown aging
sources of good 0:3 composite
Advantage - very inexpensive structure
likely to be very robust.

AGENDA

DEVELOPMENT OF NEW PIEZOELECTRIC COMPOSITES

July 24, 1989

ORGANIZERS: L. E. Cross, R. Pohanka, and D. R. Squire

CHAIRPERSON: D. R. Squire, DARPA

Overview
L. E. Cross, Penn. State

Hydrophone Performance/User Requirements
F. Geil, Westinghouse Oceanic Div.

Future Transducer Requirements
R. Ting, Naval Research Lab. (Orlando)

High Performance Piezoelectric Polymers
J. I. Scheinbeim, Rutgers University

Open Discussion with Emphasis on Implementation

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ENERGETIC MATERIALS

J. Economy, D. Squire, G. Whitesides, M. Wrighton

EXECUTIVE SUMMARY

The U.S. currently suffers from a serious conventional force deficiency which might be corrected, in part, by higher performance propellants and explosives. One application of higher performance energetic materials would be in weapons that will penetrate tank armor at greater range. Another important application of great consequence would be to lift the underwater firing restriction on the Tomahawk cruise missile. A breakthrough energetic material (discovered in 1987) is CL-20. CL-20 exceeds HMX (discovered in ~1940) in performance to an extent that dramatic improvements in military effectiveness of conventional forces weapons can be anticipated, provided that a successful production process can be developed and that the material can be stabilized satisfactorily.

HMX, currently the best high explosive, has been improved upon by CL-20 in very significant ways. One key is that the energy density of CL-20 vs. HMX is much greater, 445 vs. 109 cal/cm^3 with detonation pressures of 432 vs. 391 kbar, respectively. CL-20 represents a sufficiently large improvement in key performance criteria that large scale production is justified. The scale-up of CL-20 to ~200kg with DARPA support is critical to establishing its utility, stability, and manufacturability.

While scale-up efforts in CL-20 are underway, recent research results from SRI, International and the Naval Research Laboratory show that the properties of CL-20 can be improved upon in a surprisingly simple way. A

product of these research efforts, SRI-4, has an energy density of 584 cal/cm^3 and a detonation pressure of 449 kbar. Additional advances beyond CL-20 are thus possible and should be sought.

Two conclusions can be drawn at this time concerning CL-20: (1) CL-20 represents an opportunity to exceed parity in conventional force warfare and (2) recent research results show that properties of CL-20 can be exceeded. Additional important conclusions from a consideration of the area of energetic materials are: (1) synthesis, advanced diagnostics, and theory can be applied synergistically, to understand the keys to performance: sensitivity, shelf-life, and energy release rates; (2) limits to performance have not been established and empirical rules govern the search for new materials with few principles to guide development of materials with exceptional properties; and (3) useful energetic materials need to be viewed as a systems of oxidizer, fuel, binder, and additives. DARPA's role in the near term role is clear: focus on production of CL-20 on a scale and at a cost that will allow full evaluation in military systems. The production of CL-20 will involve the majority (~75%) of resources available. The remainder of the resources should be applied to (1) discovery and characterization of energetic materials with properties superior to CL-20, e.g., SRI-4; (2) continuation of an integrated program on synthesis, diagnostics, and theory to understand keys to performance; and (3) establishment of the fundamental foundation of energetic materials to guide the search and development of new, higher performance energetic materials systems.

ENERGETIC MATERIALS

MRC SUMMER CONFERENCE

JULY 25, 1989

James Economy[1], David Squire[2] , George Whitesides[1],
Mark Wrighton[1]

[1] Materials Research Council
[2] Defense Advanced Research Projects Agency

ENERGETIC MATERIALS

Explosives and Propellants

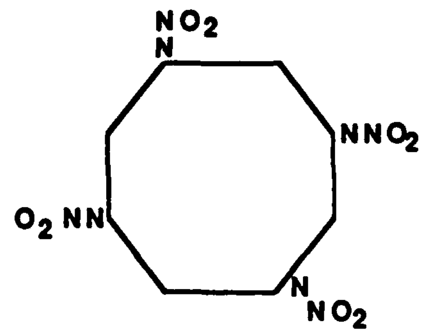
- **PROBLEM** - Serious deficiencies in conventional force capabilities may be corrected by higher performance energetic materials.

- **DOD RELEVANCE** - Weapons and rocket motors depend on energetic materials; E.g.(1) Anti-armor - greater chemical and kinetic energy penetrators - allow ~30-50% greater standoff. (2) Underwater Firing Restriction - Tomahawk cruise missile with CL-20 in booster can be launched under water.

ENERGETIC MATERIALS

Technology Status

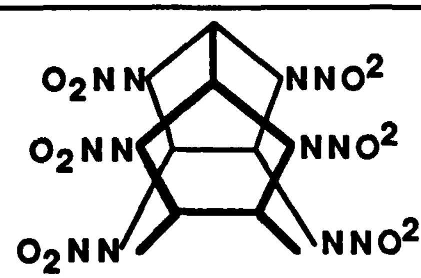
Today - HMX



109 cal^2/cm^3

- Discovered ~ 1940
- Properties: ρ = 1.90; P_d = 391 kbar

Tomorrow - CL-20



455 cal/cm^3

- Discovered 1987
- Properties:

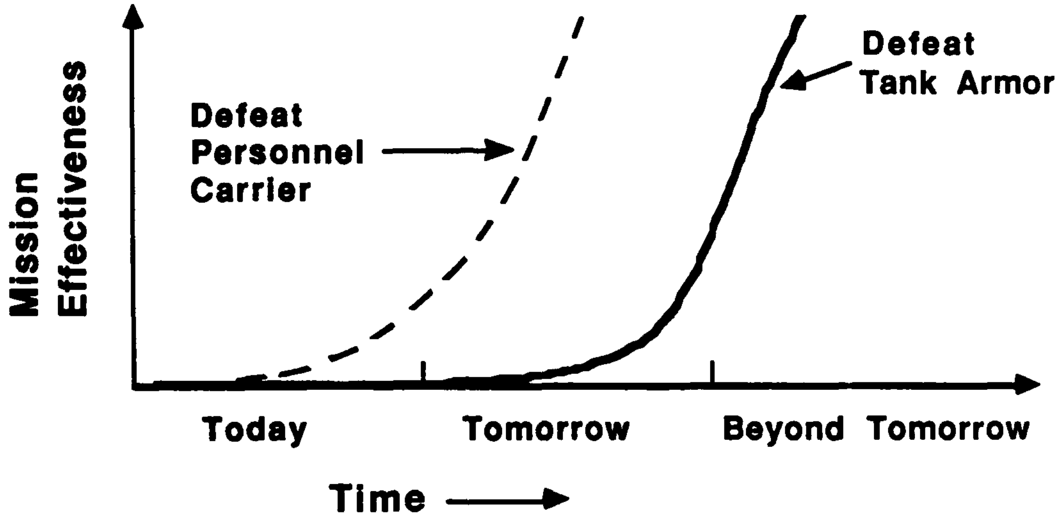
  ρ = 1.98; P_d = 432 kbar
- ~200 kg scale-up in progress.

Consequence - $\left(\frac{\rho_{CL-20}}{\rho_{HMX}}\right)^n$ n > 1 ⇒ Hyperperformance

ENERGETIC MATERIALS

Beyond Tomorrow

Rationale - Conventional Ground Forces



Beyond CL-20

Clathrate Complexes - SRI-4
- SRI-5

Cmpd.	ρ	P_d	Energy Density
HMX	1.90 g/cm^3	391 kbar	109 cal/cm^3
CL-20	1.98	432	445
SRI-4	2.015	449	584
SRI-5	2.025	456	356

1. ARE THERE NEW COMPOUNDS OR COMBINATIONS OF COMPOUNDS THAT HAVE THE POTENTIAL FOR BEING HIGH ENERGY DENSITY MATERIALS?

2. WHAT FACTORS DETERMINE STABILITY OF AN ORGANIC ENERGETIC MATERIAL?

3. WHAT FACTORS DETERMINE DENSITY OF AN ORGANIC ENERGETIC MATERIAL?

4. HOW DOES MOLECULAR STRUCTURE EFFECT SENSITIVITY, ENERGY RELEASE RATES, AND SPECIFIC IMPULSE?

5. WHAT ARE THE EFFECTS OF ADDITIVES AND MICRO-STRUCTURE ON SENSITIVITY, ENERGY RELEASE RATES, AND SPECIFIC IMPULSE?

6. WHAT EXPERIMENTAL APPROACHES SHOULD BE PURSUED TO GAIN MECHANISTIC INSIGHT INTO THOSE FACTORS THAT CONTROL PERFORMANCE AND PROPERTIES OF ENERGETIC MATERIALS? WHAT THEORETICAL APPROACHES?

7. WHAT ROLE DOES HETEROGENEITY PLAY IN DETERMINING THE PERFORMANCE AND PROPERTIES OF MIXTURES OF ENERGETIC MATERIALS?

Summary

- CL-20 represents an opportunity to exceed parity in conventional force.
- Recent research shows that properties (ρ and P_d) of CL-20 can be exceeded.
- Synthesis, advanced diagnostics, and theory can be applied synergistically to understand keys to performance: sensitivity, shelf-life, energy release rates.
- Limits to performance have not been established; empiricism is pervasive; and principles guiding development of exceptional materials have not emerged.
- Useful energetic materials need to be viewed as a system: binder, additives, oxidizer, fuel.

RECOMMENDATIONS FOR DARPA

- Focus in the near term on production of CL-20 on a practical scale.

- Continue an integrated program on synthesis, diagnostics, and theory to understand keys to performance.

- Emphasize discovery and characterization of energetic materials beyond CL-20.

- Establish fundamental foundation for energetic materials and minimize empiricism.

AGENDA AND PARTICIPANTS:

AGENDA
ENERGETIC MATERIALS
July 25, 1989

Organizers: G. M. Whitesides, M. S. Wrighton, and D. R. Squire
Chairman: M. S. Wrighton

Introduction and Overview - D. R. Squire and DARPA

Role of New Ingredients in Advanced Propellants and Explosives -
G. R. Manser, Aerojet Solid Propulsion Co.

Polycyclic Amine Chemistry - A. T. Nielson, Naval Weapons Center, China Lake

Advances in Nitration Chemistry - G. A. Olah, Univ. Southern California

Chemistry of Nitramine Propellant Combustion - C. F. Melius, Sandia Livermore

Discussion

CARS Measurements above Burning Solid Propellants - A. Echbreth, United Technologies

Highly Explosive Activated Energetic Materials - R. T. Sedgwick, S-Cubed

Spectroscopy of Shock Condensed Matter - N. Holmes, LLNL

Non-equilibrium Molecular Dynamics - W. G. Hoover, LLNL

High Energy Materials for the Future - L. P. Davis, AFOSR

Discussion

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HIGH ENERGY SYSTEMS BASED ON METAL ATOM/SMALL CLUSTER INTERACTIONS WITH HYDROGEN, CO, NH_3, ETC. IN MATRICES AT LOW TEMPERATURES

J. L. Margrave

ABSTRACT

To obtain ultimate energy-specific impulse from a fuel-oxidizer system one wants the most unstable (meta-stable) reactants which lead to the most stable products, preferably of low molecular weight.[1] Among the attractive candidates for such high-energy systems are matrix-isolated light metal atoms (small clusters) with excess hydrogen e.g., Li + H_2 or Be + H_2 which can then be oxidized (or fluorinated) to produce energy, Li_2O, some LiOH and H_2O, along with translationally hot H_2.

Another candidate metal is Ni which can form the species $Ni(H_8)$. Also, one must consider metals, like Ca, which can form $Ca(NH_3)_6$ in an ammonia matrix.

The very great chemical reactivity of clean, finely divided metal powders is well-known and easily recognized by their pyrophoric reactions in air. This potential for energy storage, to be recovered at a later time, by a controlled oxidation process can be maximized by trapping metal atoms/small clusters at low temperatures in selected matrix gases, some of which can be reactive (H_2, CO, Ch_3OH, CH_3-O-CN_3, etc.) and some of which can be inert (Ne, Ar, N_2, Kr, Xe, etc,). Initially, with Li-atoms one can identify adducts like $Li(H_2)_x$[2], $Li(CO)_x$[3], $Li(N_2)_x$[4]; Li $(CH_3OH)_x$[5,6]; $Li(CH_3OCH_3)_x$[5,6]; etc. As the interactions develop one can identify (and sometimes isolate) species like: (Li^+, H_2^-); $Li_2C_2O_2$; Li_2N_4; ($Li+LiOCH_3$); $CH_3Li+LiOCH_3$; etc. Adducts and

reaction products of Li + C_2H_2, Li + C_2H_4, Li + N_2H_4; etc. are stable in low-temperature matrices and sometimes can be isolated. [7]

In all cases, such products are spontaneously reactive with O_2 or H_2O; the presence of excess hydrogen would further enhance the potential for energy storage and ultimate utilization.

The alkaline earth metals (Ca, Si and Ba) are known to form hexammoniate solid adducts, $M(NH_3)_6$, which are metastable at room temperature.[8] In oxidizing atmospheres, these solids burn very exothermically. The existence of the $Be(NH_3)_6$ or $Mg(NH_3)_6$ analogs is uncertain but these species are probably stable in low-temperature matrices (NH_3 + H_2, for example).

In terms of energy storage there are also attractive neutral species, especially hydrides, which are "free-radicals", i.e., have an odd number of electrons. For non-metallic elements these are molecules like[9,10,11,12]:

NH_4, PH_4, etc. OH_3, SH_3, etc. FH_2, ClH_2, etc.

Usually, the species lose an electron to their surroundings and become positive ions

NH_4+, PH_4+, etc. OH_3+, SH_3+, etc. FH_2+, ClH_2+, etc

Of this group, the neutral ammonium[9-11] species is a most attractive candidate for matrix-synthesis and stabilization. For example, consider the reaction:

$$NH_4X + Li \xrightarrow{LT} LiX + NH_4$$

or

$$NH_4X + Ag \xrightarrow{LT} AgX + NH_4$$

In both cases, one would expect appreciable yields of NH_4 , and as a molecule, it should decompose very exothermically as it evolves both the recombination energies for N-Atoms and for H-Atoms. If this occurs in an oxidizing atmosphere, still more energy would be evolved.

Other "free-radical" systems to be investigated include[13,14]:

CH_5, SiH_5, etc. BH_4, AlH_4, etc. BeH_3, MgH_3, etc. LiH_2, NaH_2, etc. The alkali dihydrides are currently under investigation.[2]

Finally, the potential for forming poly-dihydrogen adducts has recently been demonstrated[15] by identification of the species $Ni(H_8)$ in hydrogen-rich argon matrices at ~10K. Isotopically labeled analogs $Ni(HD)_4$ and $Ni(D_2)_4$ -- have been spectroscopically characterized.

In summary, matrix-isolation of metal atoms (small clusters) with H_2, CO, CH_3OH, CH_3OCH_3, etc., leads to pyrophoric, high-energy products some of which can be isolated as solids at room temperature. Further exploration of selected systems is needed.

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2. X.XIAO, R. Hauge and J.L. Margrave, *Work in Progress*, Rice University, Houston, TX.
3. C. N. Krishnan, R. H. Hauge and J. L. Margrave, *J. Mol. Structure* 157, 187-196 (1987).
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5. M. Konarski, Ph.D. Thesis, Rice University, Houston, Tx., May 198_.

6. M. Konarski, W. E. Billups and J. L. Margrave, J. Am. Chem. Soc., 102, 7393 (1980).

7. L. Andrews,

8. (a)

(b)

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13.

14.

15. (a) Mingue Park, Ph.D. Thesis, Rice University, Houston, TX., May 1988.

(b) Manuscript in preparation.

BIOMIMETIC DESIGN

G. M. Whitesides, M. S. Wrighton, and I. Skurnick

EXECUTIVE SUMMARY

Purpose of the Workshop

Biomimetic design is design stimulated by cr imitating biology. This workshop examined five areas....signal processing, camouflage, sensing of gradients in chemical concentrations, biologically compatible surfaces, and fluid dynamics -- to see if the strategies used by living systems were sufficiently different from those now used in systems designed by men to provide new ideas for systems design. A number of areas of concern to the DoD -- camouflage, sonar, composites, and neural networks among them -- already show strong connections between biological and man-made systems. The question underlying the workshop was: "Could improved understanding of living systems provide ideas that could solve DoD problems?"

Conclusion

In each of the areas examined, biological systems use interesting and remarkably sophisticated strategies for solving problems in motion, sensing, signal processing, communication, detection of prey and avoidance of predators. Although each area examined generated ideas worth exploring for possible application in novel systems, biological signal processing offered the most readily implemented design principles. It is remarkable that living systems (particularly, in the context of these discussions, bats and porpoises) are able to perform signal

processing tasks that cannot presently be duplicated by man-made devices, and whose basic principles can presently only be guessed.

DoD Significance

A program in the study of biological design with the intent of identifying new principles of design, of embodying these principles in non-biological materials having properties appropriate for DoD applications, and of comparing these biomimetic systems with existing systems (if any) will lead to new strategies for robust signal processing, for robust signal processing, for jam, detection and clutter-resistant communication, for jitter detection, for sensor construction, for camouflage, and for efficient, quiet undersea movement.

Recommendations

DARPA should establish an exploratory effort ir. ``^mimetic design, teaming biological investigators with designers drawn from non-biological areas, to identify new principles used in biological systems and embody these principles in prototype devices suitable for evaluation in DoD systems. The effort should concentrate on signal processing and on sensors.

INTRODUCTION

This workshop was designed to identify opportunities to discover and transfer principles employed in biological systems to users in the DoD design/engineering community. The workshop centered around five presentations:

Richard Altes discussed strategies used in biology for signal processing. This discussion focussed on sensor fusion; on strategies for search and detector and for evasion (especially in bats, porpoises and birds); on robust algorithms for signal recovery and analysis; on clutter rejection; on jitter detection; and on cooperative communication in environments cluttered by other similar communications.

Joseph Bagnara outlined the biological basis for cryptic coloration (camouflage) in certain animal species.

Melvin Simon described the strategy used by E.Coli in detecting concentration gradients of chemicals, and in moving along these gradients in a semi-Brownian fashion.

Dotsevi Sogah summarized research relating biocompatibility to surface chemistry, using materials for small vascular grafts as an example. His talk emphasized the opportunities to use "designed" proteins and polypeptides sequences as components of biomaterials.

Thomas Daniel discussed applications of fluid dynamics in biology (blood flow, transmission of malaria, movement in fish and birds) and in population dynamics (especially the ability of different marine organisms to survive in water flow of different strengths).

BIOMIMETIC DESIGN

(BIOMIMETIC = Imitating or Simulating Biology)

Opportunity: To identify new strategies for solutions to DoD problems in signal processing, sensing, movement and camouflage, based on strategies used in biological systems to solve analogous problems.

Slide 1.

Biological systems illustrate a very wide variety of solutions to problems in motion, sensing, communication, prey detection, predator evasion and other activities having at least formal connections to warfare. The strategies employed in biological systems are constrained by the problems and opportunities in the environment inhabited by these systems. The objective of biomimetic design is to analyze these strategies and to apply them in non-biological materials and to non-biological problems. The extent to which the biological strategy can be applied to a non-biological problem varies greatly. The search and analytical strategies used by porpoises in undersea echolocation are obviously directly relevant to sonar; the biological hardware used by porpoises is not. Neural networks (as presently developed) probably have only a distant, primitive relation to the brain, but are highly stimulating to information processors. Biomimetic design is opportunistic: it searches biology for simulus at any level, from the generic to the highly specific.

CURRENT STATUS OF FIELD

- **Active science base in biology. Little connection to DoD design/engineering community.**

- **Past Examples:**

  Camouflage
  Sonar
  Composite Structures
  Drag-Reducing Polymers
  Signal-Processing Techniques
  Neural Networks

Slide 2.

Biomimetic design does not yet exist as an established field: it is an opportunity for a field, based on two circumstances. First, modern biology is in a phase of explosive growth, and is discovering new and remarkably interesting principles for the assembly, operation and control of (biological) systems. Second, the DoD faces problems whose solutions require new strategies and designs. At present, there is very little connection between modern biology and design/engineering relevant to DoD concerns.

Although biomimetic design does not exist as a structured activity, a number of examples illustrate the relevance of biological strategy to DoD concerns. Historically, camouflage and sonar were both strongly stimulated by biological phenomenon. Although composite engineering developed largely independently of biology, essentially all biological structures are composites, and most of the currently used principles of composite engineering (as well as many not yet used) are illustrated in biological systems. The use of drag-reducing polymers in ships was taken directly from biology. Methods of biological signal processing (including the broad concept of neural networks) have proved enormously stimulating in information and signal processing.

The connections between biological analysis and engineering application in most of these instances have been weak, inefficient or retrospective. There is no doubt that biology holds many strategies that would be valuable in solving DoD problems. The question is: How can relevant information concerning the design of biological systems be identified rapidly, and applied creatively, in non-biological embodiment in DoD systems?

AREAS OF OPPORTUNITY

- **Signal Processing**
  Robust signal processing, dynamic programming, sensor fusion, jitter-sensitive location, detection/location-resistant signaling, communication in cluttered environments.

- **Sensors**
  Gradient detection, motion-sensitive, damage-resistant, "Smart" or signal-processing sensors.

- **Camouflage**
  Adaptive strategies, multi-sensor resistant techniques.

- **Transport**
  Energy-efficient, low-noise (slow) undersea movement.

Slide 3.

Opportunities exist in a number of areas for technology transfer between biology and systems design. Biological systems for signal processing have a number of highly useful characteristics: in particular, they are robust (that is, they operate in noisy or cluttered environments, with missing or distorted data). They provide highly successful illustrations of sensor fusion - - The synergistic use of parallel information from different sensors (eyes, ears, touch). Biological systems have developed highly interesting strategies for signaling in ways that maximize or minimize the ease of location of the transmitter, and of operating successfully in environments cluttered by similar or identical signals. They also demonstrate certain capabilities that presently defy analysis - - for example, bat echolocation is sensitive to jitter of astonishingly small size in the target.

Biology has developed a range of sensors with characteristics that could usefully be emulated. Of particular interest are the strategies used in biology to protect sensors (for example, eyes from bright lights) and the strong propensity for biological sensors to incorporate features of signal processors and pattern-adapted matching filters.

Biological camouflage and camouflage penetration illustrates a broad range of techniques, and is not well understood. This area will undoubtedly yield stimulating concepts, especially in the area of sensor fusion.

Biological transport relies on principles almost completely orthogonal to those in man-made systems, since the wheel and rotary motors are almost unknown in biology. Analysis of these systems may suggest designs for specialized vehicles, especially for low-speed, long-endurance, low-noise undersea movement.

PROGRAM

- Establish joint biological/mechanical or biological/signal-processing teams to identify, test and compare performance of biomimetic and non-biologically derived strategies for solutions to DoD problems. Particularly promising areas are:

  Signal Processing
  Sensors

BENEFITS

- New design concepts
- New devices
- Established connections between biological analysts and non-biological designers and engineers.

Slide 4.

A program in biomimetic design should identify several areas in which new concepts in design would be welcomed by the DoD community, and establish joint biological non-biological design teams to propose, implement and test biologically stimulated design concepts. Based on current information, the most promising areas are in signal processing and sensors.

The benefits of this program would be of two sorts. First, it would develop new concepts and devices for use in DoD systems. Second, it could establish formal linkages between the biological, design and signal processing communities, and provide a new route for transfer of science from what is one of the most productive scientific communities now working (modern biology) to users in the DoD.

BIOMIMETICS AGENDA

July 26, 1989

Chairman: George M. Whitesides

Objectives: This workshop will consider opportunities in materials science, design, and signal processing.

Wednesday, July 26, 1989

George M. Whitesides; Ira Skurnick: Introduction to the workshop

Dick Altes, Chirp Corporation: Biomimetic Signal Processing
Discussion

Joe Bagnara, U Arizona: Pigmentation and Protective Coloration
Discussion

Mel Simon, CalTech: Strategies for Chemotaxis
Discussion

Dotsevi Sogah, duPont: The Biology/Materials Interface
Discussion

Tom Daniel, U Washington: Biological Fluid Dynamics
Discussion
Conclusions

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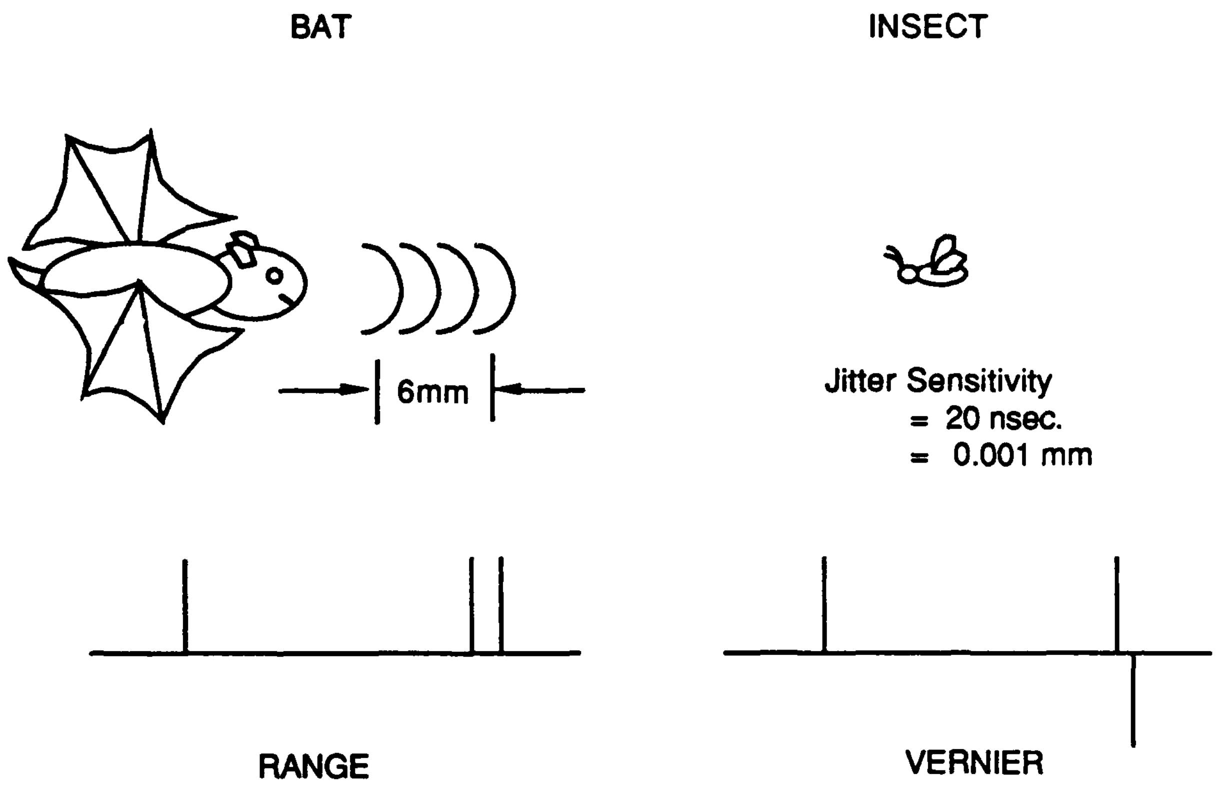
Melvin Simon	Cal. Tech.
Thomas Daniel	U. Washington
George Whitesides	MRC/Harvard
Eric Cross	MRC/Penn. State
John Margrave	MRC/Rice
John Hirth	MRC/Washington S.
John Ross	Stanford
Richard Osgood	MRC/Columbia
Larry David	AFOSR
Dick Miller	ONR
Peter Schmidt	ONR
Henry Ehrenriech	MRC/Harvard
Drew Evans	Drew Evans Assoc.
Maury Sinnott	MRC/U. Michigan
Mark Wrighton	MRC/MIT


BAT
INSECT
6mm
Jitter Sensitivity
= 20 nsec.
= 0.001 mm
RANGE
VERNIER

NEURAL NETWORKS AND CELLULAR AUTOMATA

D. K. Ferry, T. C. McGill, R. M. Osgood, B. Gilbert

EXECUTIVE SUMMARY

Artificial neural networks (ANN) and their counterpart, cellular automata, have become useful for a variety of applications. The field of neural networks has in fact blossomed into a rather large group of several thousand contributing scientists spread across a wide range of disciplines including the life sciences, engineering sciences, and physical sciences. While there are many applications in defense systems, the overall breadth of the field has hindered recognition of those tasks (from the larger volume of suggested work) that are suited to ANN. To address the former issue, a workshop was held 31 July - 1 August, with attendees from industry, university, and other government agencies. The sessions were arranged to address programs in neural network theory and modeling, implementation strategies, and real-world applications in defense related systems.

Neural networks have applications in defense systems, and can perform many of the tasks that are normally suggested for AI techniques, or intelligent operator related recognition tasks, most of which have continued to be "hard" problems in the command, control, and communications related areas. Several examples of artificial neural networks actually being used in defense systems were described during the workshop.

The current knowledge of ANN is sufficiently great that they can be applied successfully in well-posed, highly constrained problem tasks, such as static pattern (or image) recognition or dynamic adaptive (nonlinear) control

problems in some systems. The performance of these ANN will generally surpass that of alternative technologies when the application is to a problem that by nature tends to be complex and highly nonlinear, so that ordinary linear techniques are inefficient and/or smart systems are quite difficult and time-consuming to implement. Advantages that can be attributed to the use of neural networks in these areas are relatively quick implementation by one knowledgeable in the application, but not necessarily in that of neural networks, and the presence of modest learning/adaptation in the network.

The above application of current technology to defense systems should not be confused with the larger domain of researchers trying to develop a more extensive knowledge/application domain for neural networks. This latter includes specific architectures suitable for VLSI, large-scale systems, theoretical studies of the dynamics of large ANN, studies of the static attractors in the network, learning algorithms, computational theories, etc. The union of these areas should be hardware (VLSI) implemented ANN which are applicable to a number of defense system related tasks, as further understanding becomes available in each of the above mentioned scientific disciplines.

In summary, neural networks can be classified in terms of a time scale upon which research may be gauged. In the short term, there are many applications which can benefit from the use of currently understood ANN, while longer range research is required to develop new approaches. The near-term applications also provide an important feedback to the longer range programs by providing information on the capabilities of current algorithms. Generally, the long-range research should parallel the development of new VLSI architectures (and will impact these). The total field of ANN is quite broad and DARPA should

mold the program to emphasize those areas that have direct connection with defense related applications, which in the future can be expected to be architecturally based for a VLSI implementation.

Meeting Summary

The MRC meeting on artificial neural networks and cellular automata had talks from a variety of speakers on several distinct aspects of ANN. The meeting began with an overview of the programs at DARPA, ONR, and AFOSR. Mr. A. Agranat (Caltech) and Dr. D. Psaltis (Caltech) discussed the joining of optical spatial light modulators and VLSI imaging arrays to construct ANN, in which the spatial light modulators provided the connection weights for optical inputs to the summing junctions. These systems remain relatively large, in spite of the small processing chips, because of the optical path in the third dimension (perpendicular to the chips).

Dr. L. Akers (Arizona State) discussed the development of all-electronic neural nets implemented in Si VLSI. These ANN are characterized generally as lavered, locally interconnected networks due to the VLSI-imposed constraint on interconnection layers. Dr. L. Jackel (A.T.&T. Bell Labs) discussed the equivalent programs at this latter institution. The use of ANNs needs to be carefully selected due to the "steamroller of VLSI". Thus, tasks which can be performed by e.g. improved digital signal processing chips, such as linear control/filtering problems, are not good candidates for ANN. The development of ANN in Si faces a great many decision issues which relate to the choice of architecture. Normal ANN architecture usually uses very highly interconnected nodes, which is a problem for VLSI. Moreover, or perhaps as a result, the Si world does not provide very novel approaches to ANN, but tends to try to force

known ANN algorithms onto conventional VLSI. There should be an effort to develop novel architectures specifically suited to ANN.

Carver Mead (Caltech) also discussed VLSI implementations of ANN. However, he warned that the ANN area could replicate the problems of AI if not treated and guided properly, as the many thousand researchers do not currently seem to have much direction. His approach tries to use biologically inspired selections of architecture to design analog processing chips, as there is a greater wealth of information per "gate" in an analog signal. He suggested that the brain uses only 0.1 femtojoule per operation (op), while a modern microprocessor uses about 0.1 microjoule per op. Evolving fabrication technology may improve this to a nanojoule per op, but this still leaves us a factor of a million from the capabilities of the brain. While a factor of 100 may be obtained by using local interconnection topologies to overcome energy lost in interconnection lines (an architectural revolution), the remaining factor of 10K must come from a revolution in the manner in which device physics leads to operations at a node -- hence a dramatic improvement in the information content per node. He suggests that analog signals provide additional information that impacts this latter gain. The remainder must come from the temporal evolution of the signals (also analog), so that dynamic processing systems are required.

Dr. B. Haaslacher (UCSD/Los Alamos) discussed cellular automata (CA) as a new paradigm for simulation of physical systems. The CA is a discrete analog of a partial differential equation, but the dynamics are radically different than normal (finite differences or finite element) techniques of simulation. They are quite useful in special problems and but are generally terrible for general purpose computation. However, they are isomorphic to limited interconnect

ANN, and suggest certain paradigms that should be followed in developing the latter -- architectures suitable for special problems rather than general purpose.

Drs. W. Porod (Notre Dame) and T. Miller (New Hampshire) discussed the control system impact of/on ANN, particularly the stability of the system, the ability to locate basins of attraction, and the use of ANN in adaptive control systems to control robotics. Dr. R. Grondin (Arizona State) discussed the binary implementation of ANN/CA in computational structures. These talks indicated the growing awareness of the ability to design "learning" systems into conventional dynamical systems to provide improved performance in nonlinear adaptive situations. In addition, they represent the early stages of research directed to the question of how to design specific learned states a priori.

Dr. G. Works (SAIC) discussed the application of ANN in a commercial explosive detection system. Using characteristics of a thermal neutron processing system, non-experts (in ANN) were able to implement an ANN within two months, and to achieve less than 0.02 false alarm rate. Processing was done on-line with a microVax computer, thus providing real time information to the operators. He also discussed the application of an ANN to a real-time adaptive control problem of a vibration cancellation system, which provided 30 db of vibration cancellation (considerably more than the comparable adaptive filter approach).

Dr. A. Penz (T.I.) discussed the application of an ANN to signal (pattern) characterization in radar processing for an anti-radiation missile. Here, there was no possibility for prior training of the network, and ANN seems to have a significant advantage for rapid on-line training with actual data. However, if this system is to be used in real time (on a very real problem that is quite difficult) then it will be necessary to provide a 100,000 fold speedup in processing

speed, thus highlighting the need for development of special purpose VLSI hardware for the task.

Drs. L. Clarke and W. Naylor (South Florida) discussed the use of ANNs to speed-up the image processing in magnetic resonance imaging systems in medicine. Dr. T. Sejnowski (UCSD/Salk Insititute) discussed the biologically inspired model of binocular depth perception upon which he is currently working. These medical examples highlight classical difficult problems in imaging/vision which have specific applications in defense systems, but for which we currently have great difficulty in finding good solutions.

Conclusions

Artificial neural networks are useful and can currently be applied to a variety of well-posed, highly constrained problem tasks. They prove superior to other approaches, such as artificial intelligence based "smart" systems, when the task involves e.g. static pattern recognition, or dynamic adaptive, nonlinear control problems. Here, the descriptor "superior" is to be interpreted in terms of the implementation time, time to convergence, and overall cost-effectiveness of the implementation. There remain many problems, even in these areas however, such as the system response to inputs lying in the "non-trained" regions of phase space.

Research in ANN should be viewed as having a minimum of two distinct time frames. Short-range research can revolve around the application of known ANN techniques to well posed problems in real systems. Only through these approaches will definitive questions arise about e.g. the response of systems to inputs in non-trained regions of phase space, stability, and convergence problems. The application to dynamical systems will involve the extension of

current theories to incorporate a temporal base, and the incorporation of information contained in the analog signals.

The current selection of applications, for which ANN should provide improved performance, seems to center around problems characterized as complex, nonlinear mappings. These are image recognition or classification, dynamic nonlinear systems, adaptive filtering problems, etc. Even in these, it will likely be necessary that improved processing speed and power will be required, which will entail special purpose architectures, probably provided by Si VLSI. One important result obtained by the current applications discussed is that algorithms based upon the Adaptive Resonance Theory were not fruitful, as the system was not robust and was overly sensitive to small parameter variations.

Longer range research needs to concentrate on the large-scale systems aspects of ANN. One question that needs to be addressed is what is the best paradigm for these systems - biological or physical? While it may be thought that the neural concept is biologically inspired, the energy surfaces and basins of attraction come from the static physical world. The incorporation of the temporal behavior of the system suggests extended "energy" functionals, and a movement beyond just the consideration of "basins" of attraction may reveal a richer attractor structure providing more useful information content. The most mature medium in which to pursue ANN, and the one in which it will most likely be implemented, is VLSI. This provides special constraints from the quasi-two dimensional nature of its "world". Special architectural considerations should revolve around these constraints, as these have the most likely chance of high payoff for new systems and applications. Any development of ANN "computers"

is a very long range project that requires substantial interdisciplinary involvement and may require new paradigms of computation.

Recommendations for DARPA

The workshop confirmed that the DARPA program in ANN has been well formed, with efforts not only in near-term applications, but also in longer term studies addressing implementation and theory/modeling. Efforts should be made to assure that feedback from the near-term applications, concerning questions about the theory/modeling of the ANN in actual use, are made to the longer range programs. These questions concern, e.g., robustness of the ANN, response to non-trained inputs, stability, effectiveness of various algorithms, etc.

It is also fruitful to pursue implementations that are VLSI based, but also to seek novel architectures that provide enhanced performance in these implementations. Selection of longer range programs and implementations should reflect the constraint that they should be eventually useful in defense-related systems, which constrains size, weight, power requirements, etc. It is these latter constraints, along with the well-developed fabrication technology that suggests novel VLSI-based architectures for ANN is a logical direction of study.

AGENDA

NEURAL NETS AND CELLULAR AUTOMATA

July 31/August 1, 1989

Tuesday, August 1

Applications and Implementations

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ELECTROCHEMICAL POWER SOURCES

J. Economy, J. L. Margrave, D. Squire, M. S. Wrighton

EXECUTIVE SUMMARY

Current and projected military systems require electrochemical power sources (EPS). Batteries or fuel cells are used in virtually every military system requiring electric power. EPS are used in vehicles, weapons, communications, surveillance and satellites. Thus, EPS represents pervasive, critical technology.

The characteristics of EPS suggest opportunities for dramatic improvements in military systems and new EPS will allow missions not currently feasible. EPS have no moving parts and are quiet. Highly fuel efficient EPS stem from the fact that the devices are not heat engines. Some fuel cells can use a variety of hydrocarbon fuels and do not evolve pollutants. EPS are portable and modular. These characteristics suggest that advanced EPS allow signature reduction and longer mission life, while generally providing clean, safe, reliable and efficient sources of power.

An assessment of fuel cell (FC) technology reveals that the U.S. appears to be ahead, but foreigners are exploiting U.S. science and technology and gaining engineering and operating experience. Japan is estimated to be currently spending the most on FC R&D: >$100M/yr.; Tokyo Electric Power is demonstrating a 10MW H_3PO_4 FC power plant to be built by Toshiba with International Fuel Cell (IFC) cell stacks. The molten carbonate FC development in Japan represents ~2/3 of the Japan FC effort. Currently, molten carbonate FC's have the highest efficiencies (~65%) and are most versatile with respect to

fuel usage. The U.S. R&D program is funded at ~$50M/yr. with DoE providing ~$40M (~$10M to Westinghouse, ~$5M to IFC, ~$5M to Energy Research Corporation, ~$5M to M-C Power), EPRI and GRI providing ~$4M each, and DoD providing $1-2M. IFC is the world leader in sales of FC power plants; e.g., ~50-60 200kW plants sold or ordered with most sales to foreigners. European countries are actively exploring FC technology for utility and chemical plants. Total European expenditures are not known but Germany (Siemens), Switzerland (Brown-Boveri), U.K., Italy, Denmark, Holland, and Norway have an effort. Japan and European FC efforts are driven by higher energy costs than in the U.S.

In the past several years significant advances in science and technology promise rewards for new R&D efforts on EPS. These include advances in surface modification, catalysts, thin film and multilayer materials, complex ceramic structures, and new characterization tools. Siemens in Germany is exploiting proton exchange membrane (PEM) technology and Brown-Boveri in Switzerland is teaming with Ceramatek to re-start FC research on solid oxide (SO) FC's. The U.S. should capitalize on recent achievements in science and technology and develop new EPS.

DARPA should lead the U.S. R&D effort on EPS with the goal to prototype and foster commercialization of advanced EPS. A $50M/yr. DARPA-funded program leveraged by matching resources from states and relevant industries and possibly utilities would permit the U.S. to re-gain world leadership in prototyping and commercialization. Target EPS should be ones of great military value and where promising technology exists. These include solid state batteries, SOFC's, and PEMFC's. A long range effort on low temperature FC's directly consuming hydrocarbons is justified, considering

recent scientific developments and commercial impact. DARPA's investment would double the U.S. effort on EPS and markedly improve mission effectiveness while placing the U.S. in a dominant commercial posture. If successful, DARPA would propel U.S. to global technological leadership. Military benefits include new systems and lower signature and longer duration missions which are cost effective, safe, and reliable. Other benefits could include expanded commercial markets for EPS, contributions to energy independence, lower pollution energy systems, and less global warming from man's use of energy. In summary, DARPA's leadership on advanced EPS could revolutionize world wide technologies critical to U.S. economy and security.

ELECTROCHEMICAL POWER SOURCES

James Economy[1], John Margrave[1], David Squire[2], Mark S. Wrighton[1]

MRC Summer Meeting
July 10 - August 3, 1989

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THE MILITARY NEEDS ELECTRIC POWER

- Electrochemical Power Sources
    - Vehicles - unmanned underwater vehicle.
    - Communications - SUNS.
    - Weapons - ignition, propulsion, guidance.
    - Surveillance - "Silent Watch", sensors.
    - Satellites - all power needs.
    - Field Power Stations - lighting, C^3I.
- Pervasive, critical technology.

ELECTROCHEMICAL POWER SOURCES

- Batteries and Fuel Cells
  - Quiet - no moving parts.
  - Efficient - not heat engines.
  - Versatile - fuel cells accept many fuels; batteries have different shapes and sizes.
  - Portable - batteries are complete systems for conversion of chemical to electrical energy.
  - Low Pollution - not combustion devices.
  - Scalable - cells can be put in series and parallel to meet need.
- Low signature, clean, safe, reliable, high efficency power sources.

STATUS OF FUEL CELL TECHNOLOGY

- U.S. Ahead, But Europe and Japan Investing.
  - U.S. R&D - ~ $50M/yr (DOE >> EPRI ~ GRI > DOD).
    Several major contractors: Westinghouse, IFC,
    Energy Research Corp., M-C Power.
  - Japan R&D - > $100M/yr.
    10 MW Fuel Cell at Tokyo Electric Power.
  - Sales - IFC U.S. and World Leader
    50-60 200kW Power Plants mostly to foreign customers.
  - Europe - Switzerland, Germany, Holland, Italy, U.K.,
    Denmark, Norway (Military and Commercial R&D).
- U.S. research being developed by foreigners gaining engineering and o' ,rating experience.

ENABLING SCIENCE AND TECHNOLOGY

- **Breakthroughs and Achievements**
  - Surface Modification and Membrane Technology
  - Thin Film, Multilayer Materials Assemblies
  - Complex Ceramic Structures
  - Hydrocarbon Oxidation/O_2 Reduction Catalysts
  - Surface and Interface Characterization Tools
- **Advances signal opportunities for new electrochemical devices.**

RECOMMENDATION FOR DARPA

- **Lead U.S. R&D Effort on Electrochemical Power Sources with $50M/yr Program**

  - Goal - Prototype and foster commercialization of advanced electrochemical power sources.

  - Target Systems
    - Solid State Batteries
    - Solid Oxide Fuel Cells
    - Proton Exchange Membrane Fuel Cells
    - Low Temperature Hydrocarbon Fuel Cells

  - Concurrent Engineering Approach - Focus on simultaneous optimization of all components of the system; innovate "on-the-fly"; involve industry.

  - Matching Program - States and industries participate.

- **DARPA investment will result in key advances for military use and expanded commercial impact.**

PROJECTED EPILOGUE

- DARPA investment has propelled U.S. to global technological leadership.

  - Military Systems - safe, cost effective, reliable, low signature power for long missions.

  - Commercial Markets - automobiles, remote power, utilities, consumer products.

  - Energy Security - natural gas emerges as cost effective route to electrical energy.

  - Low Pollution - higher efficiency and cleaner conversion than combustion processes.

  - Lessen Global Warming Effect - more efficient use of fuel reduces CO_2 output; CO_2 can be recycled; use of nuclear power to electrolyze H_2O remotely with pipeline/fuel cell system eliminates CO_2.

- Advanced electrochemical power systems have revolutionized world scale technologies.

MAGNETIC AND MAGNETOOPTICAL RECORDING

M. R. Beasley, J. Economy, C. A. Evans, J. P. Hirth, T. C. McGill, R. Osgood and H. Ehrenreich, Chairman

EXECUTIVE SUMMARY

The magnetic recording industry is large. The U.S. annual revenue in 1989 is projected to be about $50 billion; the disk market accounts for about $35 billion. The areal information density has doubled approximately every 2.3 years since 1956. The U.S. retains a slim lead in conventional magnetic disk information storage.

A new technology, utilizing magnetooptic MO recording could be important to DoD now, and have future impact on the commercial sector. It will operate in the visible, use the same laser for both writing and reading, and overlap other DoD-driven technologies such as the search for a blue-green laser. The information storage density may be an order of magnitude greater than that for the standard technology. MO devices will have read/write capability, removable floppy disks, avoid head crashes, and be non-volatile. As in CD technology, second surface operation is possible. The primary surface passivates the active surface both chemically and mechanically.

Specific DoD applications of MO include (1) a field operable high information density floppy disk system including a monitor TV display, and information updating capability; (2) satellite-submarine communication which utilizes a blue-green laser.

R&D opportunities, which would help retain a favorable U.S. competitive position in <u>both</u> standard magnetic and magnetooptic recording include (1) the

identification of new metallic magnetic thin film alloys and layered structures utilizing a systematic characterization approach that establishes empirical correlations rapidly and helps overcome deficiencies in theoretical understanding; (2) the search for new lasers in the blue; (3) microtribology research, an essential ingredient towards understanding the dynamic head/disk interface which requires improvement, and a field that is of more general interest to DARPA in other contexts.

Finally, the US magnetic research community, which has experienced steady erosion during the past twenty years, needs rejuvenation if the goals outlined here are to be met. Evidently, this problem must be faced by research institutions and all funding agencies, not just DARPA alone.

INTRODUCTION

The magnetic recording industry is enormous. The US annual revenue in 1989 is projected to be about $50 billion, of which the disk market alone accounts for about $35 billion. The areal information density has doubled approximately every 2.3 years since 1956. While the Japanese have captured the tape-based commercial sector, the US retains an overall lead in the so-called flying head technology used in magnetic information storage. (See Fig. 1)

A magnetic recording medium consists of a permanent magnet on which a magnetization pattern can be formed along a series of tracks defined on its surface by a recording head. The schematic shown in Fig. 2 illustrates the process. The fringing field from the gap in the recording head magnetizes the medium, here simply represented as supported by a non-magnetic substrate. For a constant medium velocity, the spatial variations of the magnetization

along the track length represents the time varying magnetic signal from the head. In the reading mode, the head responds to the spatial variation of the flux emerging from the medium. At constant velocity, this variation results in an induced time-varying current. A reading head can be constructed to sense the variations of resistance with magnetic field. The use of such magnetoresistive (MR) heads has so far been restricted because of the high cost and because the variation of the resistance for permalloy (NiFe) under these conditions is only about 2%. However, new materials, to be described below, offer promise of substantial increases.

Some of the remarkable parameters characterizing the flying head technology are: Flying height (for the head), 2500A; velocity, 0.1 Mach; crash stop deceleration, 500G.

The magnetic properties of the medium and head are summarized in Fig. 3. The upper part shows the hysteresis loops characterizing the head and the disk. The recording head utilizes materials that are magnetically "soft". They have a high permeability, that is, they are easily magnetized, and have a high saturation magnetization Ms. (This is necessary because the field applied to the disk surface must be large.) They also have a low coercivity Hc, that is, the field Hc necessary to reduce the magnetization to zero, is small ($Hc < 0.5$ Oe). The remanent magnetization Mr, characterizing the value of M with the field removed, is also low. These features provide the head with the flexibility to respond rapidly to the input time-varying electric signal.

By contrast, the disk exhibits a much more nearly square hysteresis loop. The coercivity must be large ($Hc > 300$ Oe) to avoid accidental erasure. The induced voltage in the head during reading is proportional to Mr. Hence a large value of Mr is desirable.

As indicated in Fig. 3 the flying head medium structure is rather more complicated than that illustrated schematically in Fig. 2. The magnetic layer together with its undercoat are designed to optimize the medium magnetization. The overcoat, typically a carbon containing compound, must be mechanically robust to protect the magnetic data stored beneath and to minimize the damage caused by head crashes. Diamond films have been termed as "the holy grail" in the search for suitable materials. The very thin and highly proprietary lubricating layer is necessary in view of the small flying heights (which, in the future, may be reduced to as little as 500Å).

An alternative recording technology involves magnetooptics (MO), i.e., the use of laser photons to both write and read the recording medium in the presence of a magnetic field. In the writing mode, a relatively high powered laser pulse in the visible region of the spectrum raises the temperature of a magnetized medium sufficiently that an oppositely directed applied field reverses the magnetization direction locally in the heated medium, thereby encoding it as the temperature lowers. Erasure is also accomplished by a thermal process. The same laser can be used at lower powers for reading the information using the ferromagnetic Kerr effect, which rotates the plane of polarization of the probing light. When a single MO layer is used the write process must first be preceded by a separate erase step. Multilayer media show promise of obviating the necessity of this step.

A typical MO layer is shown on Fig. 3. The bracketed four layers form an interference structure. The thicknesses of the layers are so adjusted that the rotated polarization component is maximized and the non-rotated component is minimized due to interference effects.

The MO technology is potentially important to DoD at the present and could have an impact on the commercial sector in due course. (The technology

is similar to that of the CD disk in some respects; the CD disk, however, does not utilize magnetic fields.)

The importance of MO technology to DoD is that it represents a versatile, reliable, high information storage capability. It overlaps other DoD-driven technologies such as the search for a blue-green injection laser and VLSI. (At present the laser used consists of a GaAs array which is frequency doubled by materials like Nd-YAG.) Many anticipate large future growth of this technology as information processing moves increasingly into the visible. There is hope for a future US lead, even though several Japanese companies are currently ahead of IBM, the present US leader in the field. (See Fig. 1)

As indicated in Fig. 4, the MO characteristics include a high storage density, about 10 times that of flying head rigid disk storage. More importantly the MO floppy disk storage density is about the same as the hard disk flying head storage. The primary reason for this increased density, proportional to (NA/l)2, is the reduced diffraction limit in the visible region characterized by wavelength l. (The symbol NA denotes the numerical aperture of the optical system.) Since the laser can be placed some reasonable distance from the disk, which is much greater than that used in conventional magnetic recording technology, the disk is removable. Random access can be improved by introducing beam steering to replace mechanical scanning. The information storage is both nonvolatile and robust since destructive head crashes are eliminated and because, as in the case of the CD technology, the operation involves an active "second" surface that can be passivated both chemically and mechanically by a protective layer.

Specific DoD applications include a field operable high information density floppy disk system, containing, for example, detailed information

concerning the terrain and other strategically important facts that can be displayed on a small TV monitor. The disks are both robust and interchangeable. The information can be updated using the read/write mode of the system. Another possible use involves the recording of, say, satellite-submarine communication and retransmitting it, using the blue-green laser. (Note that the MO technology can utilize any wavelength in the blue; the blue-green requirement applies only to underwater communications.)

The requirements which must be met to develop this technology further are outlined in Fig. 4. The need for visible lasers is well recognized by DoD. As indicated in Fig. 3, the ideal magnetic layer utilizes an amorphous rare earth/transition metal alloy. Amorphous magnetic alloys generally have small anisotropies. As a result they should contain ingredients having large anisotropies. This issue represents both an important and physically interesting problem, since the origin of magnetic anisotropy in amorphous magnetic films is not well understood. Finally, the data rate, which is determined by the laser switching time, needs to be increased, and "archival" storage requirements, which may be short but nevertheless severe under field conditions, must be met.

As indicated in Fig. 5, there are a number of R&D opportunities to improve conventional recording technology in addition to those involving MO, just discussed. The overall magnetic thin film technology requires further development. New films containing both transition metals and rare earths must be identified systematically using the "matrix" characterization approach to be discussed in connection with Fig. 6. An exciting recent research development has shown that MBE grown FeCr superlattices having a layer thickness of about 10A exhibit giant magnetoresistance effects (about ten times larger than

permalloy). While the magnetic field and temperature conditions used to observe this effect are presently unacceptable for practical applications, it is likely that composition modifications will make such systems useful. Ways for decreasing the permeability losses at high fields and frequencies must also be sought. Since head materials tend to be mechanically soft, ways of strengthening them, perhaps by fiber reinforcement in magnetically non-invasive ways should be explored.

A corresponding set of R&D opportunities pertains to disks. The search for multilayer films having a high signal to noise ratio is a high priority item. Noise reduction can be achieved by decreasing grain size and intergranular exchange.

In view of the trends towards minimizing the flying height, and possibly even achieving an operating mode in which the head and disk are in contact, the field of thin film tribology is particularly important. The understanding of tribology on a microscopic basis is very primitive. There are many reasons, in addition to magnetic recording, for structuring a research program for exploring the fundamentals, thereby transforming an art into a science.

The last Figure summarizes recommended DARPA actions and reiterates and emphasizes the principal points in the preceding account. The topic entitled "Matrix" Characterization requires some explanation. As pointed out in the accompanying note by M. B. Beasley, which is based on his extensive experience with high temperature superconductors, we need a rapid way of preparing materials and of characterizing the relevant properties of a wide range of compositions rapidly in order to establish empirical correlations. These correlations in turn can be used to find optimal ingredients and compositions. In the case of magnetic materials this enterprise involves the

systematic exploration of a wide range of ternary and possibly quaternary alloys containing transition and rare earth metals. The Japanese are excellent in pursuing this kind of methodology. The American scientific community is, by temperament, less inclined to follow this approach unless interpretable relationships can be established quickly in the absence of theoretical guidance. The approach envisioned here is intended to overcome this impediment.

The other item requiring additional commentary concerns the US Magnetic Research Community. This community has suffered a marked decline since the mid-sixties. Universities are producing very few PhD's trained in magnetism. The Magnetic Recording Institutes at CMU and UCSD are helpful, as are one or two faculty member efforts at the Universities of Arizona, Nebraska, Illinois, Texas, and Johns Hopkins. However, they don't fill the present needs of industrial and national laboratories. This situation, which is inimical to the US competitive position in magnetic recording, is surely not one that DARPA should be expected to solve. However, DARPA should be aware of the problem and could help to ameliorate it in programs that fall naturally within its program plan.

ACKNOWLEDGEMENTS

The Study group is grateful to H. N. Bertram (UCSD Magnetic Recording Institute, J. S. Best (IBM/Almaden Research Center), and G. Prinz (Naval Research Laboratory) for helpful discussions at an informal MRC workshop on 28 July 1989. H. Ehrenreich and T. C. McGill express their appreciation to H. Sussner, D. Thompson, I. Sanders, P. Alexopoulos, D. Rugar, E. Engler and T. Suzuki for a briefing on this subject at IBM/Almaden on 12 June 1989 and to J. Matisoo and J. S. Best for their hospitality.

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- Large US Industry

  Annual Revenue (1989): $50 billion

  Projected Revenue (1990's): $100 billion

- Flying Head (FH) technology; (US ahead)

  Tape Technology; (Japanese Dominant)

- Magnetooptic (MO) Technology

  Hitachi, Sony ahead of IBM

  Important to DOD

  - Versatile, Reliable, High Storage
  - Overlaps other DOD-driven technologies

    Blue/Green Laser; VLSI

  - Anticipated Future Growth;

    Possible US Future Lead

Figure 1.

RECORDING PROCESS

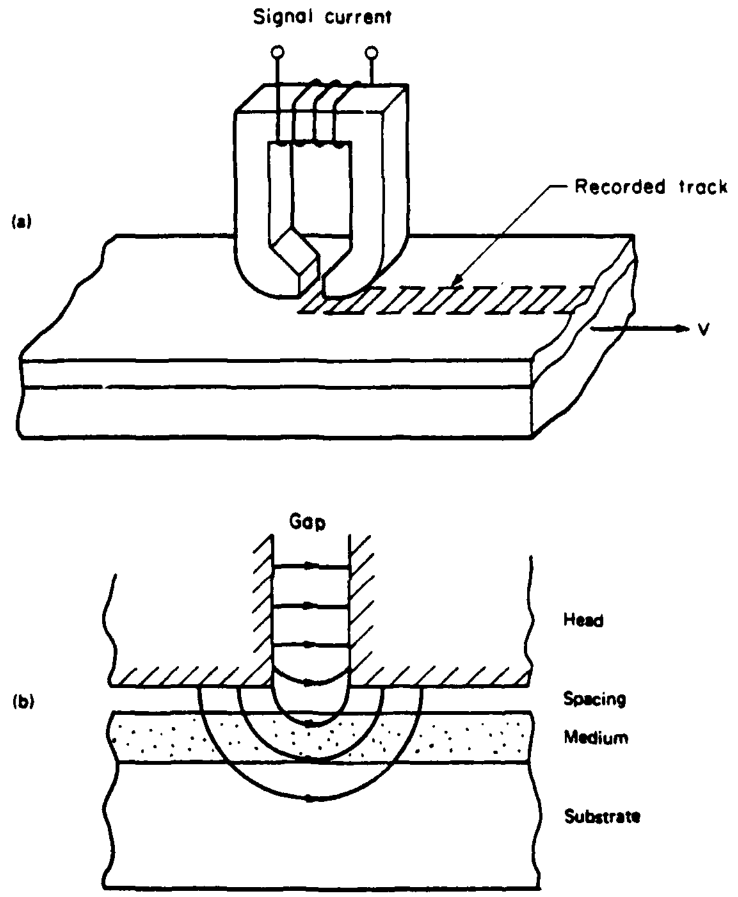
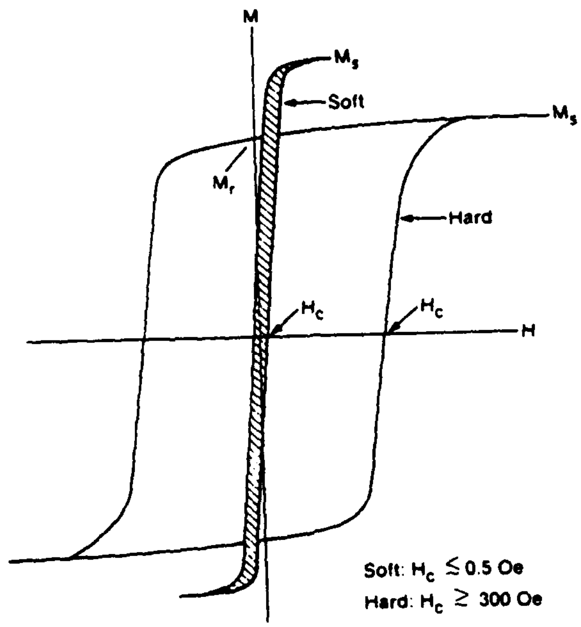


Figure 2. Illustration of the recording process using a single-track ring head. (a) Three-dimensional view; (b) cross section showing the magnetic field from the gap.

MAGNETIC HEADS, DISKS, MO MEDIA

Hard and Soft Materials: Hysteresis Loops



Heads: Soft; M_s Large; H_c < 1 Oe.
Disks: Hard; M_r Large; H_c > 300 Oe.

<u>Medium Structure</u> <u>Flying Head</u>		<u>Magnetooptic</u>
Lubricant (.1nm)		Overlayer (120nm Quartz)
Overcoat (30nm -- diamond?)		Magnetic Layer (15nm a-RE/TM Alloy
Magnetic Layer (Co-based)		Intermediate Layer (80nm Quartz)
Undercoat (10's nm Cr)		Reflector (50nm Al)
Substrate	BOTTOM	Substrate

*Multilayer Interference Structure

Figure 3.

MO Characteristics

- High Storage Density ~0.5 Mb/mm^2; ~ $(N_A/\lambda)^2$; ~ 10x Flying Head
- Removable Disk, Random Access, Displays
- Read/Write
- Nonvolatile, Robust: Eliminates head crashes
- Uses Visible Light, wavelength λ ~ 320 - 530 nm
- Second Surface Operation (CD technology)
- Beam Steering can replace Mechanical Scanning

Needs

- Visible 30-100 mW Lasers (Blue-Green!)
- Advanced Multilayer films: MO Alloy/Mag. Anisotropic Alloy
- Increased data rate (>> 5Mb/s)
- Archival storage requirements

  $\Rightarrow$ Corrosion resistance, low chemical reactivity, improved overlayers

Figure 4.

R&D OPPORTUNITIES

- Meet MO Recording Needs

RECORDING HEADS

- Thin Films
  - Transition Metals/Rare Earth Metals (CoZr)
- Multilayer/MBE grown Superlattices
  - Giant Magnetoresistance Effects
- Low Loss permeability
  - High fields; high frequencies (>100 Mhz)
- Mechanical Toughness

DISKS

- New Ternary and Quaternary Alloys (CoPtCr)
- Advanced Multilayer Films
- Noise Reduction: decreasing grain size and intergranular exchange
- Decrease corrosion; improve mechanical properties

HEAD/DISK INTERFACE

- Thin Film Tribology

Figure 5.

RECOMMENDED DARPA ACTIONS

- Encourage "Matrix" Characterization

  for Optimal Medium/MO/Head Properties

  - Establishes empirical correlations

  - Overcomes deficiencies in theoretical understanding

- Search for New Visible Lasers

- Emphasize Microtribology Research

- Help rebuild US Magnetic Research Community

Figure 6.

PHOTONIC MANUFACTURING

A. Yang, A. Yariv, C. M. Stickley

Executive Summary

The optoelectronic - or photonic-industry in the U.S. is large, variegated, and growing. Our study sought to identify the segments of this industry which are most important to DoD applications and where the U.S. is in danger of falling behind. We believe that within the broad area of photonics the area of semiconductor laser sources is the most vulnerable and vital technology to meet this criterion. While the other critical components and arrays such as modulators, switches, and connectors etc. are still in conceptual design stage that should be included in the initiative at a later stage. These laser sources are the root (enabling) components in a large number of DoD and civilian applications which include:

(1) High speed data recording, retrieval, and communication
(2) Space communication
(3) Computer interconnect and supercomputers
(4) Visible light sources and pumping of solid state lasers for communication with submarines
(5) Phased array radars, microwave delay lines and antenna remoting
(6) Fiber gyroscopes for munitions, navigation
(7) - Mostly civilian - fiber to the home.
(8) Optical signal processing (radar, solar, images)

The U.S. is in good shape and in some cases, ahead, as far as Research and Development of these lasers are concerned but very likely will lose the market to the Japanese in spite of the lead. This is due to the fact that efficient low cost manufacturing will come with big volumes and big volumes depend on availability of reliable inexpensive laser and laser systems. Japanese companies are moving up the learning curve due to their involvement in large volume markets, a number (5-7) of which include: compact disc laser (1.8×10^7/yr), Laser printers, Optical data storage, cameras (range finding).

RECOMMENDATIONS

To break the vicious cycle of large volume manufacturomg low cost lasers, DARPA should set up 2-3 pilot plants for generic semiconductor lasers. The emphasis should be on flexible manufacturing and automated packaging and testing. The candidate lasers should be those with potential for large volume applications and could correspond roughly to those shown in the figure. The situation is still early enough so that a well chosen intervention by DARPA at this stage could make a real impact.

APPLICATIONS

(1) High speed data recording, retrieval, and communication

(2) Space communication

(3) Computer interconnect and supercomputers

(4) Visible light sources and pumping of solid state lasers for communication with submarines

(5) Phased array radars, microwave delay lines and antenna remoting

(6) Fiber gyroscopes for munitions, navigation

(7) - Mostly civilian - fiber to the home.

(8) Optical signal processing (radar, sonar, images)

MEETING REPORT

The study on photonic manufacturing was undertaken to address a number of concerns:

(1) Are there critical DoD requirements for optoelectronic components?

(2) Is the U.S. losing its technological lead in optoelectronics (photonics)?

(3) Is U.S. industry going to be frozen out of key segments of the photonic market?

(4) Are there critical system requirements of DoD which will depend on foreign based suppliers. (This assumes that the answer to question #1 is positive).

An earlier study undertaken at the request of Michael Kelly of DARPA and involving two of us (Yang, Stickley) as well as representatives from industry identified a large number of technology areas important to DoD in which photonics will play an important role. These include Telecommunication, Light Sources, optical components, optical test equipment, lasers, sensors/detectors, displays, imaging technology, modulations, materials.

As a first step we decided that it is important to narrow the above list down and identify those technologies which are central to as large a number of DoD applications as possible and which are most at risk. The area which we

identified as meeting these criteria is that of semiconductor diode sources. The centrality of three different types of these sources to a large number of DoD and civilian applications is illustrated in Figure 1. The figure illustrates how semiconductor lasers (CL's) are the root component which enables the following applications:

1. Space communication
2. Printing
3. Optical Data Storage
4. Frequency doubling to obtain blue-green sources for underwater communication.
5. Medical endoscopic applications
6. Bragg cells for Radar signal spectral analysis
7. Smart weapons
8. Local area networks
9. Microwave transmission over fibers
10. Microwave signal distribution for phased array radars.
11. Visible light sources (obtained by pumping solid state lasers by diode arrays) for submarine communications.
12. Machining and trimming machine parts and electronic circuits.
13. Optical interconnect
14. Optical signal processing

The schedule of the meeting and a list of the invited speakers is attached.

A. Yang opened the meeting with a description of DARPA's interest and concerns in the photonic area and an explanation for the choice of

semiconductor diode sources as the "root" enabling technology for the photonics industry.

M. Stickley described and summarized previous meeting organized by DARPA's Defense Manufacturing Office to look into the problem of photonic manufacturing.

A. Yariv in his introductory comments made the point that U.S. Research and development in diode sources is more or less on par with the Japanese with one serious exception - development of visible semiconductor diodes where the U.S. effort is almost non-existent. The U.S. is far behind is in laser manufacturing. Japanese companies with large internal markets for compact discs and in the optical data storage are moving up the manufacturing learning curve and are in danger of dominating in the future other segments of the markets.

Another aspect of the U.S. - Japan race pointed out by A. Yariv is the asymmetry of the competition. Companies with total sales, volume of $20-40 billion in Japan (Hitachi, Toshiba, Matsushita.....) on one side and scrappy U.S. companies with annual sales under $20 million (PCO, Lasertron, ORTEL, Spectra diodes) on the other. The implication of this asymmetry in terms of the ability to invest in automated manufacturing and to ride out lean times is obvious.

Some issues raised by the participants were:

Don Scifres, Spectra Diodes

(1) U.S. industry is highly fragmented because we lack a consumer industry. Spectra Diodes as an example is continuously asked for small numbers of specialized components.

(2) There are no customers willing to invest in 6.2, 6.3, 6.4 type programs.

There is lack of appreciation in customers and DoD for investments in reliability cost reduction and in manufacturing. Don Scifres of Spectra Diodes described how MITI is funding two companies to develop semiconductor lasers for pumping solid state lasers to the total tune of $40 million over 3-4 years. The basic technology was developed by his company.

Another example of U.S. technology that is in danger of Japanese domination is ORTEL'S window laser for high power applications and its ultra low threshold lasers whose research stage was funded by DARPA. In both of these instances the initial research effort in the U.S. was not followed by the necessary development and manufacturing effort due to the smallness of the companies and the lack of coordinated national support.

R. Smith of AT&T Bell Labs commented that because of the division at AT&T into numerous smaller profit centers the corporation no longer throws its full weight behind product development and manufacturing.

I. Ury - ORTEL

Emphasized, again, the fragmentation of the U.S. market due to lack of high volume consumer electronics markets. In contrast to laser markets in compact discs, printers, optical data storage, and cameras in Japan. He pointed out that potentially U.S. can have high markets in fibers to the home (POTS, HDTV, etc.) computer interconnects and phased array radars. To supply these markets U.S. companies will need to set up low cost high volume and efficient production lines.

Jim Goell of PCO re-emphasized some of the above points especially lack of support and resources for manufacturing technology and the fact that

U.S. is being outspent in the area of product development, not research.

R. Chang, Hewlett-Packard told us that his company is the world largest supplier of semiconductor optoelectronic components - mostly the relatively inexpensive display type devices. His company is only interested in volume (>1 million/yr) production and because of it can invest the relatively large sums required to design dedicated manufacturing lines.

The single most consistent theme to emerge from the meeting was that the U.S. is far behind in high volume low cost manufacturing of reliable semiconductor diode sources. This situation will lead, if uncorrected, to foreign industries, domination of major segments of the photonics market-U.S. prowess in research not withstanding.

It was also agreed that the best way to break into high volume production is for the U.S. Government to help set up a small number of pilot lines with emphasis on efficient low cost manufacturing. Each participant had his own preference of what items should be the subject of these first pilot lines. There was a general agreement, however, that one should emphasize generic products with a potential for large volume markets. The committee in its post meetings deliberation chose the following main products as candidates for pilot lines:

(1) High power (>100mw) GaAs/GaAlAs semiconductor lasers.

(2) "Low" power (1-5mw) GaInAsP lasers.

(3) Incoherent High Power (>1 watt) GaAs lasers for pumping of SS lasers.

(4) Basic transmitter-receiver modules for Avionics data, computer interconnects, HDTV, etc.

The range of potential applications for each of the above sources is depicted in Figure 1.

Our main conclusions were:

1. It is important for the U.S. to develop a manufacturing capability in laser source and basic receiver/transmitter modules.
2. These are important DoD requirements for sophisticated optoelectronic components.
3. There can be no advanced U.S. industry in basic and sophisticated photonic sources which will have only DoD as a major client.
4. U.S. companies are either too small or unwilling (!) to invest in large scale efficient photonic manufacturing (Hewlett-Packard is an exception but only in the low end relatively unsophisticated part of the market).
5. U.S. government action is needed to help U.S. companies become large volume manufacturers.
6. With the exception of AT&T the best laser source technology in U.S. now resides in small (< $\$2x10^7$/yr) companies.
7. DoD should launch ~3 pilot lines for low cost efficient high volume manufacturing choosing *generic* products with potentially large markets.
8. Candidate products for such pilot lines are a number of basic laser sources which were listed above and possibly laser basic transmitter/receiver modules.

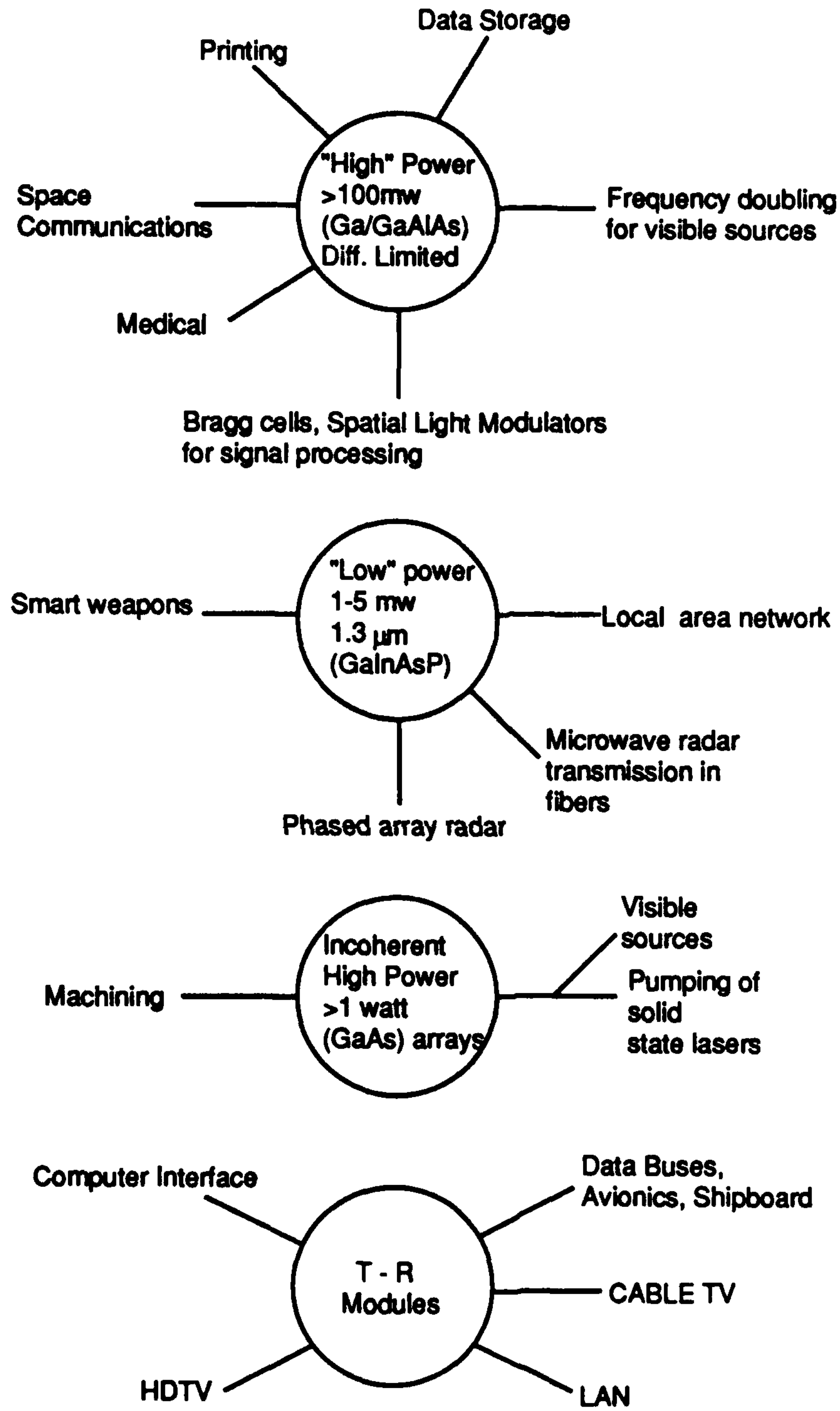

Data Storage
Printing
"High" Power
>100mw
(Ga/GaAlAs)
Diff. Limited
Space
Communications
Frequency doubling
for visible sources
Medical
Bragg cells, Spatial Light Modulators
for signal processing
"Low" power
1-5 mw
1.3 μm
(GaInAsP)
Smart weapons
Local area network
Microwave radar
transmission in
fibers
Phased array radar
Incoherent
High Power
>1 watt
(GaAs) arrays
Machining
Visible
sources
Pumping of
solid
state lasers
Computer Interface
Data Buses,
Avionics, Shipboard
T - R
Modules
CABLE TV
HDTV
LAN

Figure 1.

AGENDA

U.S. PHOTONIC MANUFACTURING

July 19, 1989

<u>Wednesday, July 19</u>

1:00 PM	A. Yang (DARPA)
	A. Yariv (MRC/Caltech)
1:30-1:50	D. Scifres, Spectra Diodes
1:50-2:10	R. Burnham, Amoco
2:10-2:30	I. Ury, ORTEL
2:30-2:50	J. Goell, PCO
2:50-3:10	R. Smith, AT&T Bell Labs.
3:10-3:30	Coffee Break
3:30-4:30	Panel Discussion
4:30-5:00	Summary of Conclusions

BIOTECHNOLOGY

George M. Whitesides, Mark S. Wrighton

The promise of commercial biology - that is, biotechnology - is ultimately based on the development of extraordinary techniques that make it possible to decipher and to modify the genetic information coded in cells, and thus to trace and control the mechanisms of biosynthesis (especially of proteins) and of cellular and organismic differentiation and development. The first products of biotechnology, and those on which much of the original enthusiasm for the area was based, are proteins -- insulin, human growth hormone, tissue plasminogen activator, interferons and interleukins, and now erythropoietin and related compounds. Certain of these compounds will undoubtedly be important (even revolutionary) pharmaceuticals, but current analysis of the area of biotechnology suggests that they (and other proteins) will <u>not</u> ultimately dominate the pharmaceutical market. They will undoubtedly provide a relatively small number of durable products. More importantly, they will provide <u>leads</u> for the development of conventional drugs. The ultimate drugs, in this view, will continue to be classical chemical entities, and the most important influence of biotechnology will be to improve the efficiency with which these materials can be developed. Biotechnology will also provide cells, organs and animals as products. The importance and market potential of these products is not presently defined.

The U.S. developed molecular genetics and biotechnology, and enjoys a strong lead in these areas, especially in protein engineering. The techniques of molecular genetics are, however, generic, largely non-proprietary and freely available internationally. Thus, of the three geographical areas currently

technically active in biotechnology and advanced pharmaceuticals - the U.S., Western Europe, and Japan - the ultimate beneficiary will be the one most efficient at using biotechnology in whatever way is appropriate to develop new products. In this application of biotechnology the U.S. still has a strong lead, but has no intrinsic protection for its lead. In the technologies related to scale-up of biological products -- reactor control, metabolic, isolation, ultrapurification -- it is probably inferior to Japan. It suffers, moreover from four serious current non-technical disadvantages. First, the cost of regulatory clearance of a new drug in the U.S. is very high, and the time to reach market large. Second, product liability issues make it unattractive for U.S. manufactures to address any but the largest markets. Third, the pharmaceutical industry is bracing for a wave of hostile takeover activity; this activity has severely damaged the technical competitiveness of other areas of the U.S. manufacturing sector. Fourth, the availability of capital for small company operation, one of the driving forces behind the U.S. biotechnology industry, has been severely limited by the market collapse of October 1987 and by changes in the capital gains tax structure.

Although there are significant technical problems facing the current generation of protein products, particularly the development of techniques for ultrapurification of proteins, the rate of development of the field is such that the DoD can therefore play an important role in problems requiring long-term solutions. In brief, the DoD could make major contributions to the long-term health of commercial biotechnology in five areas:

1. **Advanced Computation**

Biotechnology is now generating information at a rate far beyond the capacity of biology and medicine -- both, by tradition, non-mathematical areas -- to absorb. The techniques for data-base management, pattern recognition, signal processing, and advanced scientific computing developed by the DoD community could, if transferred into commercial biotechnology, make an enormous difference in the speed with which the field could move from research to products. A particularly important long-term (10-20 year) problem is the so-called "rational drug design" problem: that is, the use of crystal structure information for enzymes or receptors to design, de novo, clinically effective drugs that bind tightly to those proteins. This problem will depend critically on computation for its solution.

2. **Cell Culture**

One set of the next generation of products of biotechnology will be human cells (for use both auto- and allografts). Certain of these products will be directly relevant to major DoD concerns in trauma. The initial products in this area are now being introduced by small companies. Cultured human skin for use in treatment of burn is the most advanced of these products. The DoD could speed the development of this technology by funding research in the supporting technologies (laser wound preparation, cell preservation, cell shipping and storage) and by providing protected markets for these initial market entries.

3. **Biomaterials**

There is a large market for non-biological materials for use in living systems. The design of these material, falls clearly within the capabilities of the materials technologists in the DoD community.

4. **Biomimetric Design**

Biomimetic design is the analysis of the principles by which living organisms accomplish their requirements in movement, sensing, control, and communication, and the transfer of these principles, when appropriate, into non-biological embodiments. (An example would be a silicon-based signal processor for echolocation designed to follow some of the principles of signal processing used by bats). Although not presently a part a bio-technology, biomimetic design could be of great value of the DoD in providing new types of devices and systems.

5. **Product Scaleup and Purification**

In the current generation of biotechnology products (especially proteins), scaleup is a critically important problem. Certain areas -- ultrapurification of proteins; "smart" chromatography, electrophoresis, dialysis; sensors and sensor fusion in fermentation control-- would rely on DARPA's strengths in materials, sensors, and control.

JET ENGINES

R. Mehrabian, J. C. Williams, W. Barker

EXECUTIVE SUMMARY

The pre-eminence of the American jet engine is founded upon unprecedented performance and reliability. It is the result of technological innovation coupled to unique manufacturing methods which, heretofore, have been exclusively the products of American enterprise. With global industrial frontiers shrinking rapidly, foreign concerns (notably the European aerospace consortium and the Japanese) are attempting to penetrate the jet engine market in order to uproot the base now controlled by U.S. engine manufacturers. The strategies which are being brought to bear appear to be threefold: 1) copying, to eliminate the costs of development; 2) introduction of improved machining methods, to reduce the cost of manufacturing of an otherwise equivalent product; and 3) development of new technologies based on new materials and processes, to produce a product of superior performance. It is in the latter category that DARPA can play an important role to assist the American propulsion community meet the global competitive challenge.

Advances in the level of performance and efficiency of the modern gas turbine engine are generally paced by the capabilities of materials used in their construction. There are two schools of thought for meeting materials requirements for high performance/lightweight compressors, combustors, turbines and exhaust nozzles. The first, would concentrate efforts on evolutionary technologies based on conventional materials (nickel-based superalloys, titanium, etc.) and incorporate new processing and manufacturing

technologies. The second, would tend to "skip over" the next generation of metallic materials and develop a host of new composite materials for future generations of aircraft propulsion systems. Programs that have been initiated based on the latter approach include the DoD Integrated High Performance Turbine Engine Technology Initiative (IHPTET) and the NASA Advanced High Temperature Engine Materials Technology Program (HITEMP). NASA program is primarily an in-house research activity (80% of FY88 R&D Funds).

Needless to say the United States must pursue both avenues through manufacturing technology initiatives for use of existing and evolutionary materials, and as well as programs for development of advanced composites. It should be noted that incorporation of complex new materials in jet engines is going to be very difficult and will require coordinated efforts between the materials, design and fabrication communities. Furthermore, lack of experience-based design data is a major obstacle. DARPA can play an important role in both preserving the competitive edge for the next generation of military engines (e.g., the ATF) and their commercial spin-offs, and the establishment of a model design and manufacturing capability for production of sophisticated advanced materials components.

In particular, DARPA should support technology-base activities for improved monolithic materials components through programs such as the following:

- Concurrent engineering - to reduce the time and cost of new designs. This can build on the DICE concepts and programs.
- Process modelling and control activities which build on and expand the impact of the Intelligent Processing of Materials (IPM).

DARPA's support for new materials for significantly improved performance (e.g., doubling the capability of the future generation aircraft propulsion systems) should again focus on advanced processing concepts to reduce cost and produce sufficient quantities of these materials to demonstrate feasibility through use in perhaps static components. Duplication of efforts already underway (e.g., NASP, IHPTET, and HITEMP) should be avoided. DARPA programs could include:

- Development of continuous processes for tailored metal matrix composite (MMC) systems based on both relatively mature monolithic metal alloy matrices and advanced alloy matrices such as titanium aluminides.
- Application of DICE and IPM concepts from conventional materials systems to composites.
- Coordinate efforts of microstructure design community (i.e., URI programs) with manufacturing (materials suppliers) and engine producers (e.g., GE, P&W, Allison, Garrett, Lycoming) to develop necessary design protocols based on experience in non-man-rated threatening applications.

U.S. AEROSPACE IMPORTANCE

- Sales of $112 billion
- Contribute $15 billion annually to positive side of trade balance
- Employs more than 1.3 million workers
- Broad economic impact - purchases from 34 different industries
- Aerospace defense equipment - 50% of 1987 defense procurement budget
- Aerospace is key element of civil transportation system

3M ALUMINA FIBER

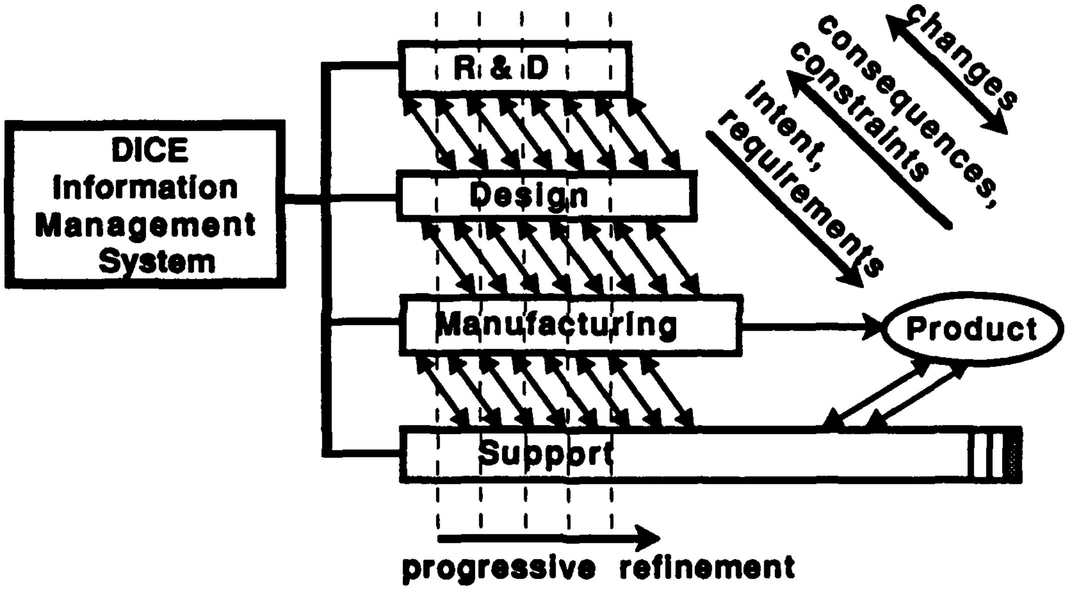
- 99% Alpha Al_2O_3
- Tensile strength 300-400,000 psi
- Elastic modulus 55×10^6 psi
- Use Temperature 12-1300°C
- Scale up process $50/lb.

	HITEMP	IHPTET
FOCUS	Civilian Engine Materials (6.1)	Components for Military Aircraft (6.2, 6.3)
MAJOR MATERIAL EMPHASIS	800 F PMC 1500 -2500 F IMC 2000 -> 3000 F CMC 2800 F-Nb Alloy	Very High Temperature -Al, Ti, Ni & Refractory Alloys High Temperature PMC C/C Advanced Intermetallics Tix Aly Composites Non-Structural Materials
MAJOR DRIVERS	Est. 2500 hrs. at Max. Temp. per Year 2900 Hrs. Utilization Per Year Long Time Interdiffusion Creep, Oxidation, TMF Mach Range 0.6 to 4.0	Est. 65 Hrs. at Max. Temp. per Year 250 Hrs. Utilization per Year Light Weight, High Temperature, HCF, TMF Mach Range 0.6 to 3+ Sustained
FINAL OUTPUT SOUGHT	Demonstrated Composites Feasibility by 1992	Technology Demonstrated in 1990-2000 Time Frame to Provide 100% Increase in Thrust/Weight Ratio -50% Decrease in Fuel Consumption

DARPA Initiative in Concurrent Engineering

DICE

A Systematic Approach to Rapid Product Development



RECOMMENDATION

- DARPA should not duplicate NASA's HITEMP OR DoD's IHPTET programs

- A two pronged approach is needed:

  1) Improve monolithic materials jet engine manufacturing technologies through DICE and IPM type programs.

  2) Select one process (perhaps continuous) and generic composite material (e.g., titanium-based MMC) to produce sufficient materials and products to gain experience and develop design and processing protocols.

- Exploit DICE and IPM approaches in the MMC program as well as university-based (e.g., URI) microstructure design concepts.

RELATIVE REACTION RATES OF METHANE VS. ACETYLENE IN THE FORMATION OF CARBON-13 DIAMOND THIN FILMS

C. Judith Chu, Robert H.Hauge, Mark P. D'Evelyn, and J. L. Margrave

ABSTRACT

Carbon-13-labeled diamond films were synthesized by hot-filament-assisted chemical vapor deposition. Mixtures of $^{13}CH_4$ and $^{12}CH_4$ in H_2 were used with a total hydrocarbon concentration of 0.5% in H_2. The first-order Raman frequency at 1332 cm^{-1} for ^{12}C-diamond was found to shift by 50 cm^{-1} to 1282 cm^{-1} for pure ^{13}C-diamond. The diamond peak is also found to shift linearly within these limits as a function of the ^{13}C mole fraction. This linear correlation has been used to study the relative reaction rates of methane versus acetylene.

The incorporation of ^{13}C-methane was compared to ^{12}C-precursors by investigating the ^{13}C-mole fraction of the resulting diamond thin film. Concurrent investigations of the gaseous species generated during the hot-filament-assisted CVD of diamond by matrix-isolation FTIR spectroscopy indicate that the ^{13}C-mole fraction in the resulting diamond thin film correlates with the ^{13}C-mole fraction of the methane in the gas phase and not that of the acetylene.

This leads us to conclude that under filament-assisted CVD conditions, methyl radicals derived from methane are primarily responsible for diamond growth.

EXPERIMENTAL

A Schematic diagram of the heated-filament-assisted chemical vapor deposition chamber is shown in Figure 1. CVD diamond thin films were grown on tungsten substrates using a variety of hydrocarbon precursors such as methane, acetylene, isotopically labeled ^{13}C-methane and acetone in H_2. Growth rates of approximately 1.75 microns per hour were achieved with the following experimental conditions:

W filament temperature - 2000-2100°C

substrate temperature - 800-950°C

chamber pressure - 24-27 torr

percent hydrocarbon in hydrogen - 0.3-1.0%

filament to substrate distance - 7-10 mm

gas flow rate - 100-200 sccm.

All gases were of research grade, 99.99% purity, with the exception of $^{13}CH_4$ which was 99.3%. Gas flow was controlled by mass flow meters. The temperature of the tungsten filaments was monitored by an optical pyrometer and that of the substrate by a Pt/Pt10%Rh thermocouple.

Characterization of the CVD diamond thin films was obtained using Raman spectroscopy and x-ray diffraction. The presence of crystalline diamond has been positively identified by both techniques. Raman spectra were obtained on a Spex Raman spectrometer employing 488 nm Ar-ion laser excitation. Carbon-13-labeled diamond films have also been grown using mixtures of $^{13}CH_4$ and $^{12}CH_4$ in H_2. Gaseous species near the substrate were sampled into gas bulbs via a water-cooled copper collection tube to be subsequently analyzed by matrix-isolation FTIR spectroscopy.

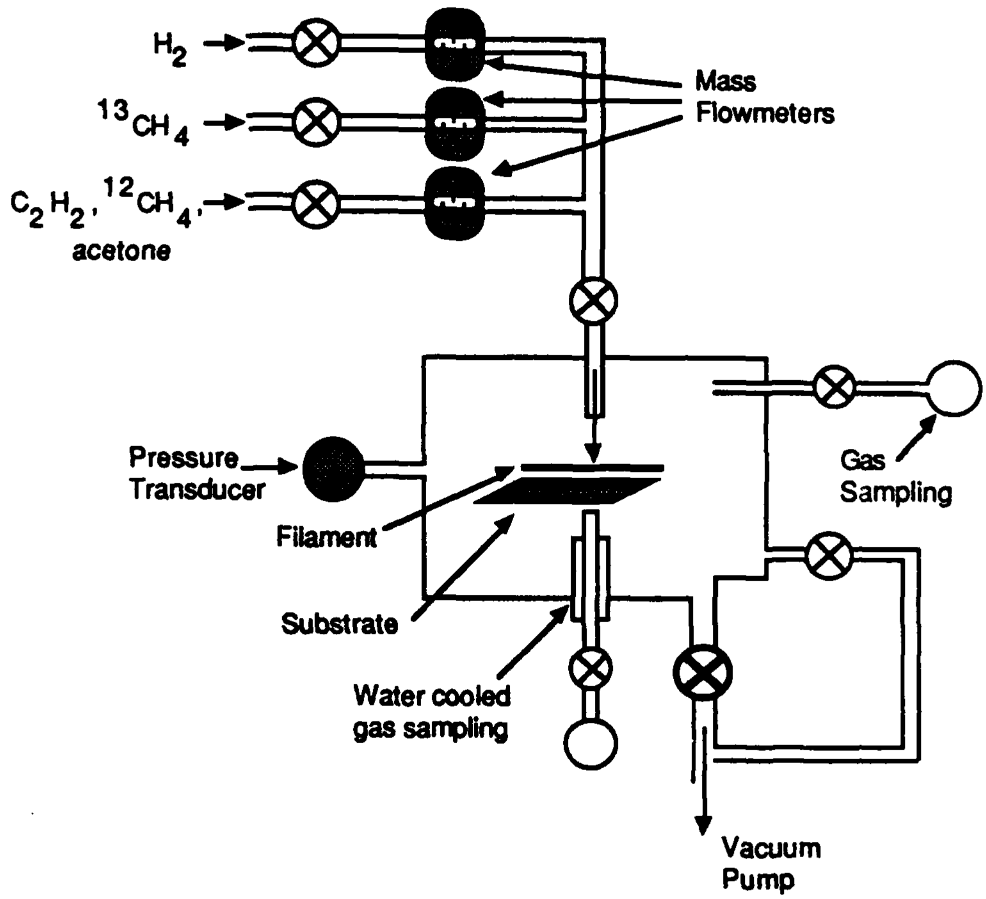


Figure 1. CVD Chamber

RESULTS

Linear Correlation Between the First-Order Raman Shift of Diamond and C-13 Mole Fraction

Carbon-13-labeled diamond films have been grown using mixtures of $^{13}CH_4$ and $^{12}CH_4$ in H_2. Raman spectra of the films are shown in Figure 2. The Raman peak at 1332 cm^{-1} for ^{12}C-diamond is found to shift by 50 cm^{-1} to 1282 cm^{-1} in pure carbon-13 films and the peak shifts linearly between these limits with the ^{13}C mole fraction. A plot illustrating this linearity is shown in Figure 3 with the corresponding frequencies and ^{13}C mole fractions listed in Table I. The fact that only one single peak is observed for the first-order Raman spectrum of the mixed diamond films indicates that ^{13}C and ^{12}C isotopes are homogeneously distributed in the diamond crystals, as has also been noted by Chrenko.[1]

The Raman shift for the pure ^{13}C-diamond film can be calculated using the equation of monatomic lattice vibrations and assuming the existence of a mass effect, i.e.,

$$\omega = (4C_1/M)^{1/2} \, |\sin Ka/2|$$

where

ω = frequency

K = wave vector

C_1 = force constant between planes

M = mass

a = spacing between planes.

By substitution, this reduces to

$$\omega_1/\omega_2 = (M_2/M_1)^{1/2} \text{ and}$$

$$\omega_{C\text{-}13} = \omega_{C\text{-}12}\,(12/13)^{1/2} = 1280 \text{ cm}^{-1}.$$

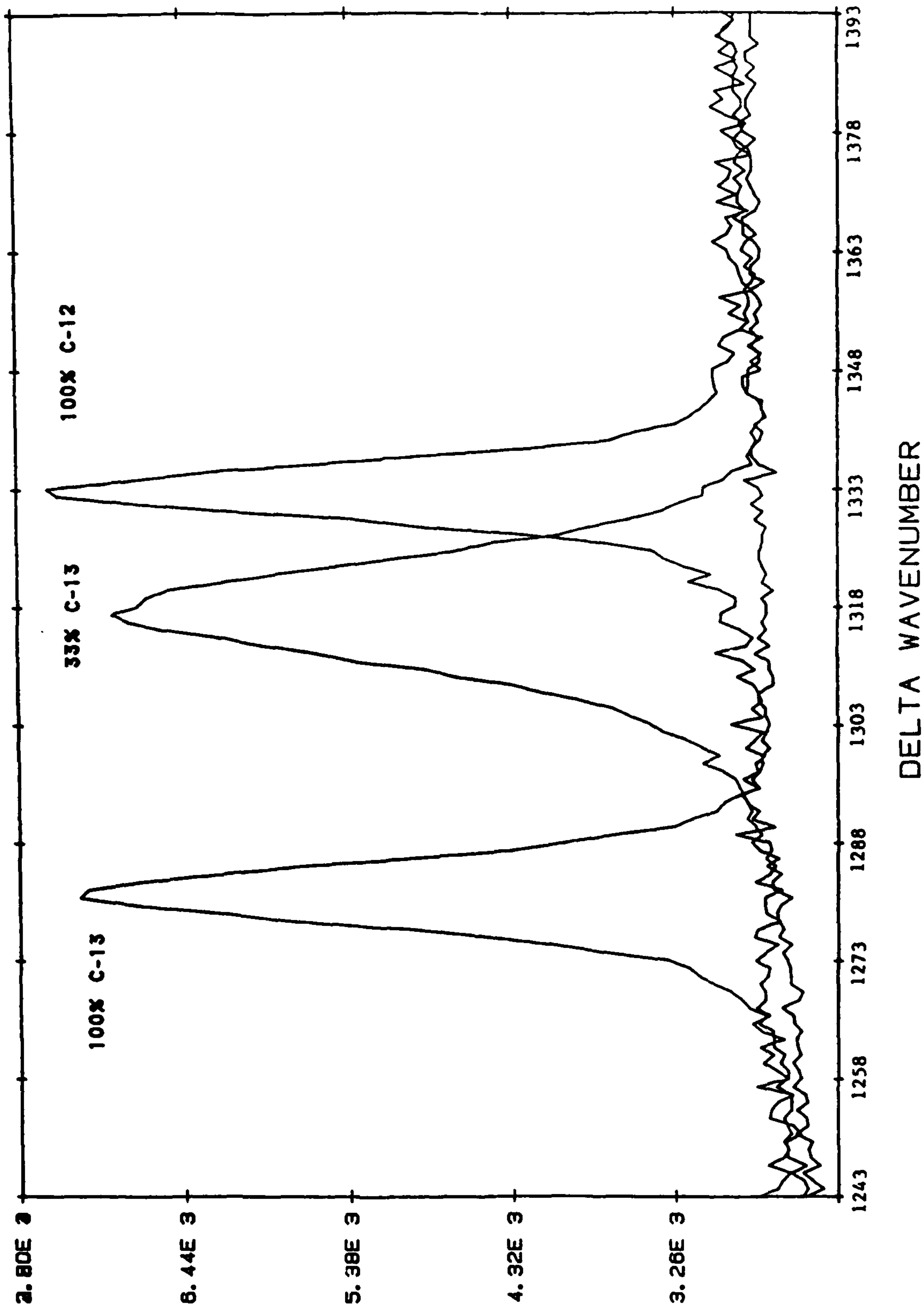


Figure 2. Raman Spectra of ^{13}C-Diamond Thin Films.

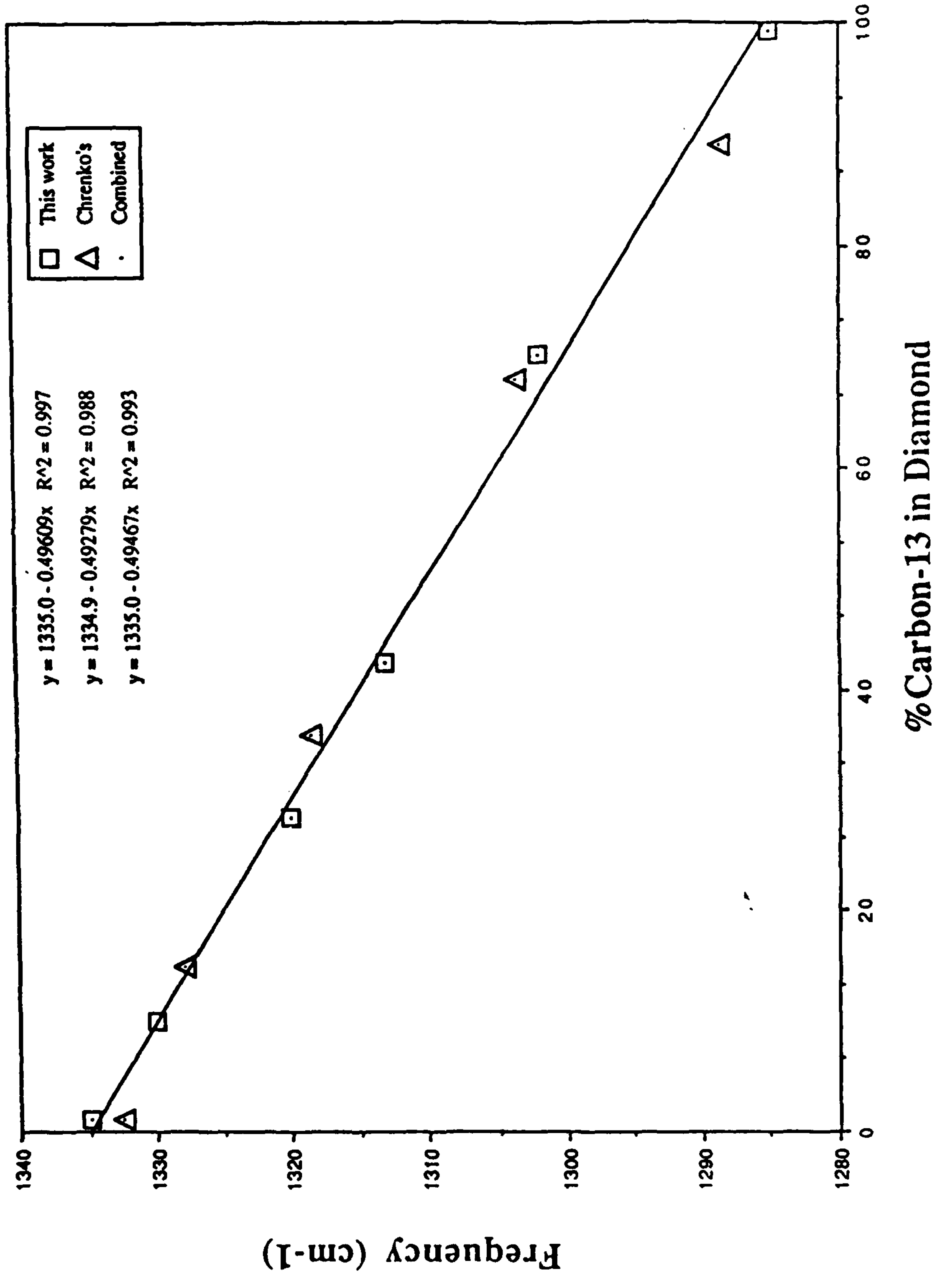


Figure 3. Effect of C-13 Mole Fraction on the Raman Shift of Diamond.

TABLE I. Raman Frequency for Carbon-13 Diamond Thin Films

% Carbon-13	Raman Frequency (cm^{-1})	Bandwidth (cm^{-1})
99.3	1285	9
70.2	1302	15
42.6	1313	15
28.4	1320	14
10.0	1330	15
1.1	1335	5

This calculated Raman frequency of 1280 cm^{-1} closely approximates the experimentally observed value of 1282 cm^{-1}.

The observed linearity between the Raman frequency and ^{13}C mole fraction allows a direct comparison of the incorporation efficiencies of different growth precursors with isotopic labeling. For example, growth studies using $^{13}CH_4/^{12}C_2H_2$ mixtures and $^{13}CH_4$/acetone mixtures yield information concerning the relative reactivities of methane versus acetylene and acetone where isotopic mixing is incomplete.

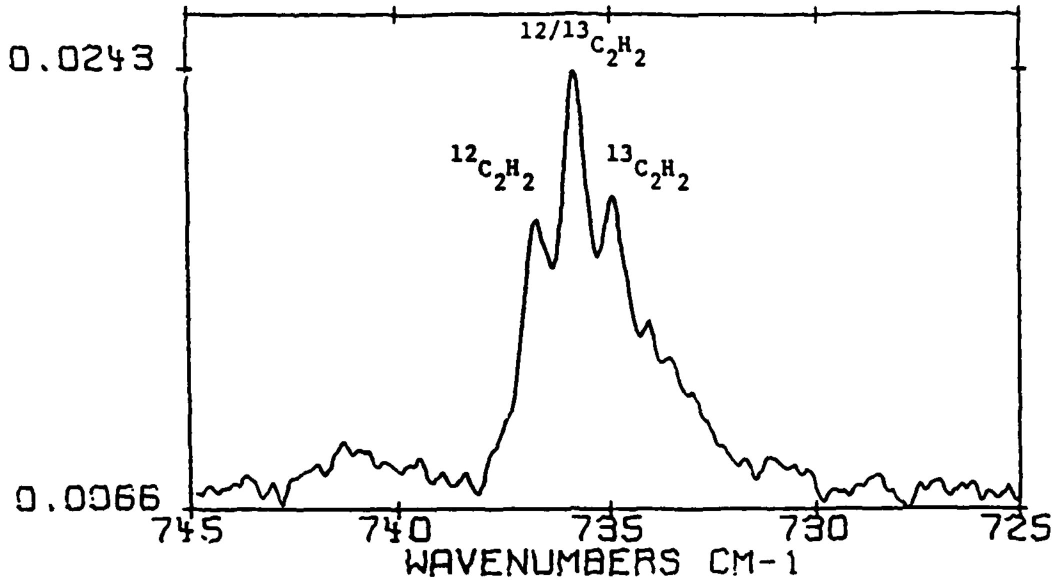
Relative Reaction Rates of Methane Versus Acetylene in Diamond Formation

Growth studies using isotopic mixtures of $^{13}CH_4$ and $^{12}C_2H_2$ and $^{13}CH_4$ and ^{12}C-acetone were performed. Results of these studies are tabulated in Table II which lists the reactants, the ^{13}C percentages of the resulting diamond film, the initial reactants, and the methane and acetylene which were sampled during reaction at the diamond growth level.

Table II. Comparison of % Carbon-13 in the Initial Reactants, Measured Diamond, and Gas Phase Methane and Acetylene.

	% Carbon-13				
Reactants	Initial Reactants	Measured CH_4	Measured Diamond	Measured C_2H_2	CH_4/C_2H_2
17%$(^{12}CH_3)_2{}^{12}CO$ 83% $^{13}CH_4$	62 ± 3	67 ± 3	62 ± 2	75 ± 5	3.6
37%$(^{12}CH_3)_2{}^{12}CO$ 63% $^{13}CH_4$	36 ± 3	39 ± 3	36 ±2	50 ± 5	6.0
33% $^{12}C_2H_2$ 66% $^{13}CH_4$	50 ± 3	50 ± 3	50 ± 2	65 ± 5	4.9
23% $^{12}C_2H_2$ 77% $^{13}CH_4$	63 ± 3	60 ± 3	60 ± 2	45 ± 5	4.0

The relative concentration ratios of methane and acetylene present in the gas phase are also given. Analysis of the gas phase with matrix isolation - FTIR spectroscopy indicated only methane and acetylene are present as major stable species in the gas phase. Percentages of ^{13}C in methane and acetylene were determined from peak height calculations of methane and acetylene infrared absorptions as illustrated in Figure 4 for 37% acetone and 63% $^{13}CH_4$. The methane/acetylene ratios were calculated based on an acetylene extinction coefficient of 4.5 times that of methane.



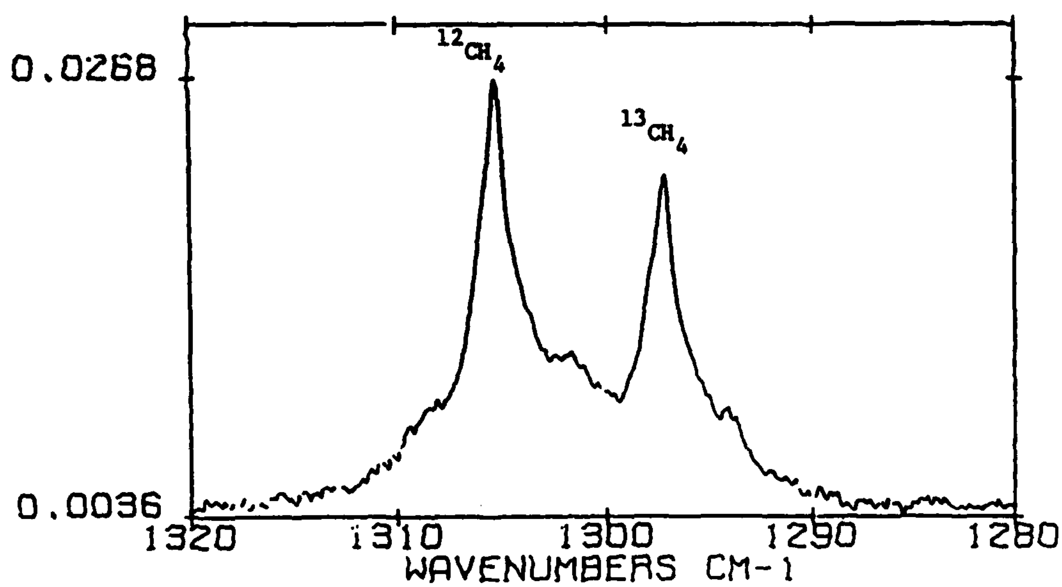


Figure 4. Matrix Isolation FTIR of Gas Phase Species.

Observations and conclusions from the experimental data are:

1. All carbons of methane, acetylene and acetone are available for diamond formation with acetylene acting as a two carbon donor and acetone as a three carbon donor. It is also concluded that all carbon atoms are reduced to methane since the isotopic C-13 percentages of the measured methane match those of the initial reactants.

2. Formation mechanisms of acetylene do not allow it to achieve isotopic equilibrium with methane in the gas phase.

3. The measurement of the methane/acetylene ratio is approximately 4 to 1 in agreement with Butler, et. al.[2]

4. **The measured methane C-13 percentage agrees with that of diamond while that for acetylene does not. Since the isotopic ^{13}C percentage of methane should closely approximate that for the methyl radical, the above agreement indicates that the methyl radical is the primary carbon source for diamond growth.**

For instance, taking the example in Table II where the initial reactants are 33% C_2H_2 and 66% $^{13}CH_4$, if methane and acetylene were equally reactive and the methane/acetylene ratio is 4.9 then, the expected ^{13}C percentage in diamond is 54, i.e.,

$$\frac{\text{(C-13 fraction in methane) } 4.9 + \text{(C-13 fraction in acetylene)} 2}{4.9 + 2}$$

$$= \frac{(.5)\ 4.9 + (.65)\ 2}{6.9} = .54$$

If acetylene is twice as reactive as methane then the expected C-13 percentage in diamond is 57, i.e.,

$$= \frac{(.5)\,4.9 + (.65)\,(2)\,(2)}{4.9 + (2)\,(2)} = .57$$

Thus one concludes that methane is at least as if not more reactive than acetylene. Also since it is known that the methyl radical is approximately 400 times less abundant than methane, its relative reactivity mist accordingly be at least 500 times that of acetylene with respect to diamond formation.

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FREE-STANDING DIAMOND SHAPES--
CYLINDERS, HEMISPHERES, GRIDS AND FIBERS

C. J. Chu, R. H. Hauge, J. L. Margrave, D. E. Patterson

ABSTRACT

One can imagine many practical applications for large specific shapes of pure diamond deposited on preforms which allow subsequent transfer of these diamond shapes to any other material of the same shape. As we now have an improved understanding of the low pressure processes for growing diamond thin films, techniques for growing specific cylindrical, hemispherical, parabolic, and elliptical shapes are being developed. These shapes have clear cut potential uses as low friction and low wear bearing surfaces as well as very scratch resistant coatings for mirrors and lenses. Hemispherical diamond radomes are also of interest. One might like to have a diamond wear stripe on a cylinder part. It is difficult to predict which structural uses of diamond composites will prevail, but it is clear that a large number of interesting possibilities exist.

Technology which will make optimum use of the new low pressure diamond growth process remains to be developed, i.e., rapid deposition of smooth, high-quality diamond on relatively cool substrates. Current diamond growth chemistry requires deposition temperatures of ca. 900°C. The diamond film is often not strongly bonded to the substrate, and the upper growth surface is always rough and multifaceted. One can actually take advantage of the rough surface by making it the bonding surface, thus providing enhanced physical bonding. This allows one to expose the smooth underlying surface for

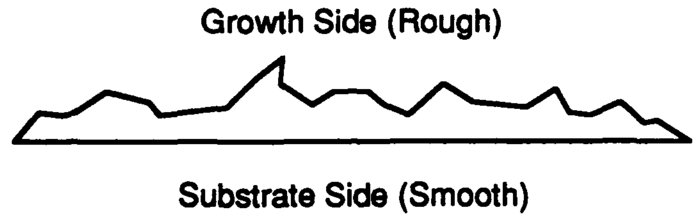
use as a low friction, low wear bearing surface. Low temperature bonding methods also allow for the attachment of smooth diamond coatings to a much larger range of materials. Creating defined diamond shapes and bonding them to other materials is at the heart of new diamond application technologies.

INTRODUCTION

In the last four years both American and Japanese investigations have demonstrated that diamond films can be grown at low pressures on substrates such as silicon, copper, tungsten, etc.[1,2,3,] Typically, the films are a few microns thick and multicrystalline in nature. In a few cases, films of almost 1 millimeter thickness have been grown. Diamond film growth is reported to be most rapid on substrates held at temperatures near 900°C, and growth rates in the range of microns per hour are typical. Low pressure chemical vapor deposited (CVD) diamond growth is commonly achieved using a gas mixture of approximately 99% hydrogen and 1% methane. Other hydrocarbons such as acetone and acetylene have also been employed as the feed gases as have other carbon containing species such as carbon monoxide. A necessary requirement in this form of diamond growth is the production of hydrogen atoms. This is accomplished by passing the gas mixture through a microwave or RF discharge or, alternatively, over a hot tungsten filament (>2000°C) or through a flame. It is thought that the hydrogen atoms serve to assist diamond growth kinetically by forming both free radicals on the growth surface and gas phase hydrocarbon radicals. Hydrogen atoms are also thought to play an important role in removing any graphitic material that is formed since it is known that graphite is preferentially etched by hydrogen relative to diamond. In fact, the formation of graphite is known to be excessive when the percent of methane (or

other carbon source) in hydrogen reaches levels on the order of 3% or more. This effect currently places an upper limit on diamond growth rates.

Ultimately, the use of diamond films as practical coatings will depend on whether they can be grown on or transferred to substrates of choice such as drills, saws, shafts, optical materials, etc., with strongly adhering properties. In some cases, the rough growth surface which results from the multicrystalline nature of the diamond films is also not desirable. This is true if one desires a hard low-friction surface. Typical diamond film morphology is illustrated below.

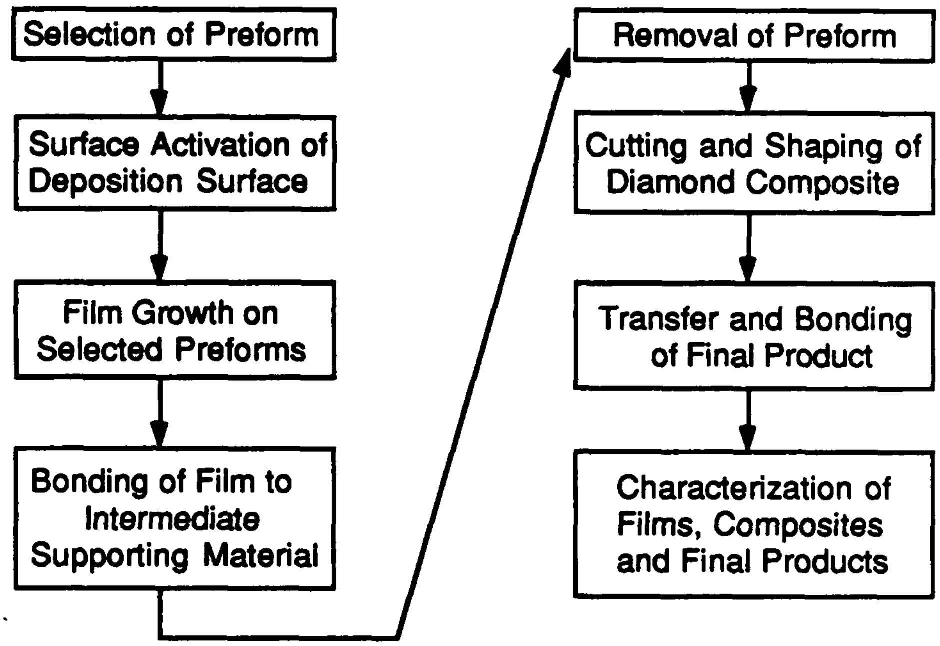


The rough side of CVD diamond films has also been found to be extremely difficult to polish. A final consideration is that in many cases the materials which can benefit the most from a diamond coating cannot withstand the 900°C temperatures without losing some of their desirable properties, e.g., hardness. Very recent reports describe diamond growth on silicon substrates at ~320°C[4].

Techniques for Growing and Utilizing Free-Standing Diamond Films.

Significant steps associated with thin film diamond materials processing are outlined by the following flow chart.

Diamond Film Processing



Since a cylinder is of broad general usefulness, consider the formation of one inch by one inch thin walled diamond cylinders. In using a preform, free-standing diamond cylinders can be grown with the rough side either on the exterior or interior of the cylinder depending upon the deposition apparatus. Schematics for forming free-standing CVD diamond cylinders are shown in Figure 1.

The hot filament technique is most commonly used initially as all growth parameters can be easily controlled. The flame/plasma jet techniques potentially provide higher growth rates but still require more development effort. One can use preforms to produce thin walled spheres, ellipsoids, hemispheres, paraboloids, wires or filaments, and grids. Each of these diamond shapes

Free-Standing CVD Diamond Cylinder Apparati

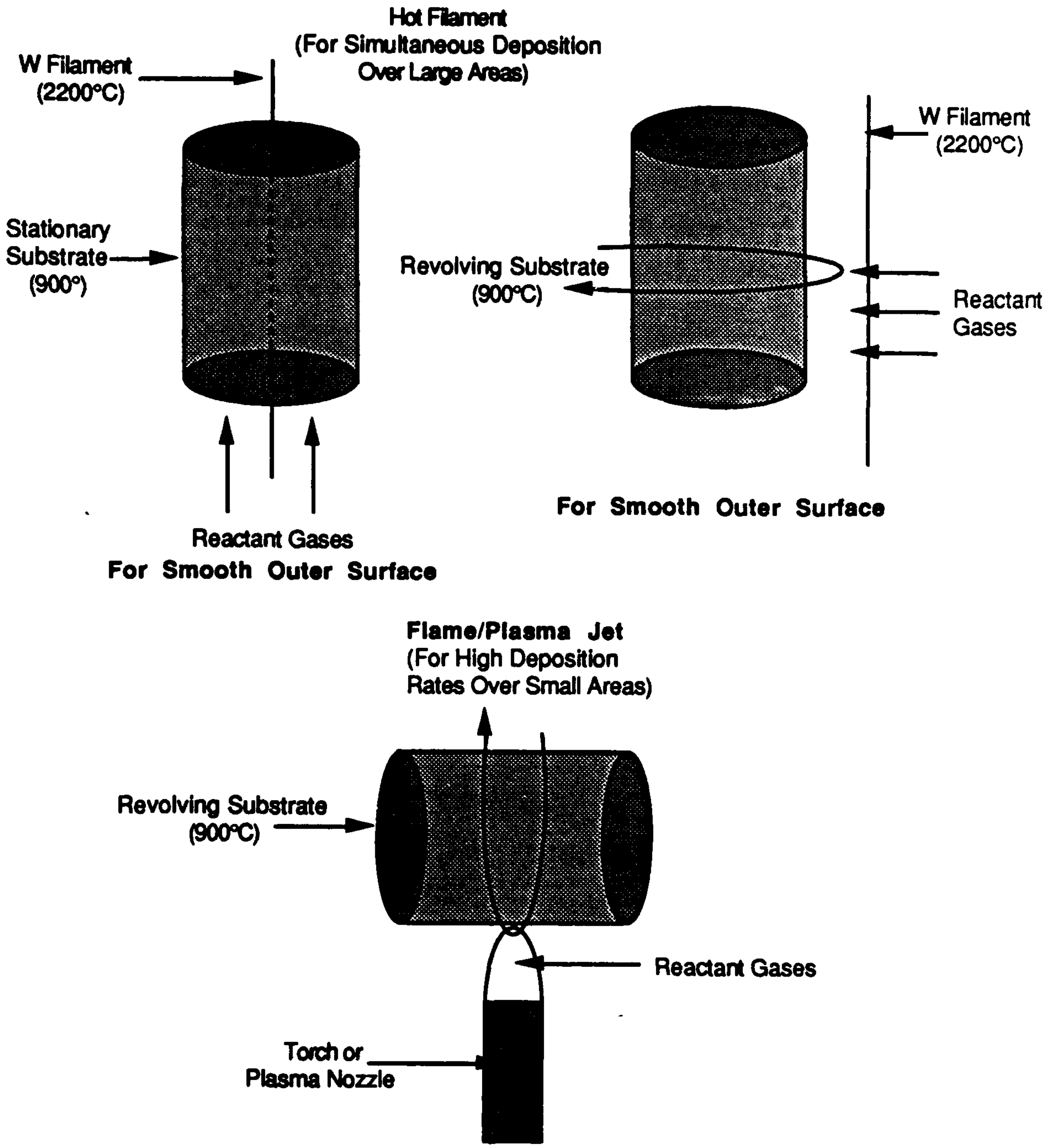


Figure 1.

could prove useful when transferred and bonded to a final product. In general, preforms must have their surfaces activated prior to diamond film deposition. This activation is often carried out by rubbing the surface with ordinary diamond polishing grit (typical grit size is less than 1 micron). Larger diamond pieces or diamond knives may also be used to scratch the deposition surface if a particular diamond growth pattern is desired.

The mechanisms by which carbon adds to the growing diamond surface are the subject of current basic research studies at Rice University as well as elsewhere. In some studies in our labs, isotopically pure ^{13}C diamond films have been prepared to study growth mechanisms.[5] The two most prevalent theories suggest that the methyl radical[3] or acetylene[6,7] is the active carbon species which adds to the diamond surface. Gas phase probes find both species are present in sufficient concentration to act as the active species but recent findings in our labs have shown that the methyl radical is the dominant growth species. We have also developed a unique mixing technique which does not expose the hot filament to hydrocarbons. This has been shown to give maximum deposition rates with minimal graphite contamination in the diamond films. It is also believed that this technique precludes metal contaminants from the heated filament from being introduced into the diamond film.

In bonding the diamond films to other objects, one can take advantage of the rough growth side of the film to attach an intermediate support physically to the diamond film. This support material can then be bonded to shafts, optical surfaces, etc. Intermediate supporting materials are usually metallic and can be bonded to the diamond by a variety of techniques. CVD deposition of an intermediate metal support material can be achieved by introducing the proper metal halide into the diamond deposition chamber with excess hydrogen

following diamond growth. Another possibility is to sputter-coat the diamond film using established metal sputtering techniques. Direct physical bonding of the rough side of the diamond films to liquid metals, plastics, and glasses is also possible.

Many uses of diamond films involve separating the film from the preform to take advantage of diamond's optical transparency, mechanical strength, hardness, etc., without being limited by the preform substrate material or the high substrate temperatures required for formation of a diamond film. One recently developed technique for separating thin films from substrates makes use of elemental fluorine as the chemical agent.[8] The ease and completeness of separation is dependent upon the deposition substrates and the relative volatility of its fluoride. Also, metal substrates can be electrochemically removed to leave free-standing diamond shapes. If necessary, the freed diamond "composite" can be trimmed before transferring to another material.

The transfer and bonding of the diamond composite is the final step in placing the diamond coating on or in a finished product if, indeed, the diamond composite is not the final shape itself. This can be achieved in several ways depending upon the desired final product. In many cases, the diamond composite may be attached using common adhesives to such materials as plastics and glasses. For instance, extremely hard, inert coatings could be placed on optical materials by carefully matching indices of refraction between the coating and the original material. Electrochemical plating techniques may be employed to further add a variety of metal coatings to the diamond composite. Soldering techniques can also be used to attach the composites to metals.

Another interesting application of the diamond composites is the direct deposition of diamond films on fibers or wire grids (again made of silicon, carbon, silicon carbides, refractory metals, etc.). These diamond fibers or grids could then be used as the fiber reinforcement for metallic composites. Thus, diamond fibers, directionally woven or chopped, might be placed in aluminum or aluminum-magnesium alloys to achieve stiffening and strengthening.

A large growth area for diamond films is believed to be in the semiconductor industry. As diamond has anywhere from 2 to 4 times the heat conductance of any metal at room temperature and has extremely high electrical resistance, diamond films or diamond composites should make superior heat sinks. For proper evaluation, it will be essential to measure the heat conductance and resistivities of the diamond materials. Diamond fiber reinforced metal composites can be tested for improved tensile strengths, stiffnesses, and other mechanical properties. The diamond films themselves can be evaluated for purity using Raman spectroscopy, X-ray diffraction, and scanning electron micrography. Cylinders of diamond may also be of interest in chemical reaction systems where the diamond cylinder defines the region where critical reactions occur.

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SPECTRAL EMISSIVITIES OF LIQUID TRANSITION METALS AS FUNCTIONS OF TEMPERATURE AND WAVELENGTH

S. Krishnan, G. P. Hansen, R. H. Hauge, J. L. Margrave

ABSTRACT

Ellipsometric methods have been utilized to measure optical constants, reflectivities and emissivities of both solid and liquid transition metals which are heated and levitated in a radio frequency induction core. The spectral emissivities (a = 488, 514.5, 632.8 and 1064nm) for Cu, Ag, Au, Ni Pd, Pt and Zr were observed up to ~600°K above the melting points.

INTRODUCTION

Many of the fundamental properties of liquid transition metals are poorly known, especially at temperatures above 1500°K. For example, spectral emissivities are important from the standpoint of determining the thermodynamic temperatures of molten metals/alloys by the use of optical pyrometry. Ellipsometric methods have been utilized to make measurements of spectral emissivities and dielectric constants of both solid and liquid refractory metals which have been heated by the use of electromagnetic levitation thus avoiding container interactions. The results indicate moderate temperature dependence of the spectral emissivities for liquid Cu, Ag, Au, Ni, Pd, Pt, and Zr for superheats up to 600°K above the melting points. Further, the spectral emissivities of the liquids were found to be higher than the corresponding solids while those of the undercooled liquid appeared to be virtually the same as that

of the liquid above the melting point. Excellent agreement was seen with available literature data for both the spectral emissivities as well as the optical constants at the melting point.

Spectral emissivities are of fundamental importance when one wishes to carry out reliable radiation measurements of temperature[1-8]. The questions addressed in this study are; 1) Do spectral emissivities depend on temperature above the melting point? 2) Do spectral emissivities vary as a function of wavelength? and, 3) Is the temperature dependence different at different wavelengths?

The use of ellipsometry for measurement of the optical properties of solid and liquid metals is not new[9-18]. However, the use of this technique for emissivity measurements on the refractory liquid metals and alloys as a function of temperature above their melting points is novel. One difficulty in handling very refractory liquid metals is that they are highly reactive. However, this problem is eliminated in the current experiments with the use of an electromagnetic levitation system where the liquid drops are completely isolated from any containers. The levitation technique also has other attractive features such as the ability to control and vary temperatures so that one can study solid emissivities by resolidifying the liquid (this produces very clean surfaces). With the use of this arrangement, it has been possible to measure solid and liquid metal optical constants and emissivities in the temperature range 1000-3000°K quite easily. The highest temperature is usually dictated by the vapor pressures of the material being studied and the coil designs that are used.

We present here optical property measurements, including spectral emissivity, as functions of temperature at wavelengths of 488, 514.5, 632.8 and

1064nm for a number of electromagnetically levitated liquid metals including Cu, Ag, Au, Ni, Pd, Pt, and Zr. The data include measurements on liquids, solids and undercooled liquids. Complete experimental details can be found in other publications[19-25]. The above metals were electromagnetically levitated and melted, and rotating analyzer ellipsometry[10] was performed on the light reflected from the sample.

The liquid spectral emissivities of the copper and nickel groups are plotted in Figs. 1 and 2, respectively. It is seen quite clearly that the spectral emissivities increase gradually with decreasing wavelength, until the blue region where a sharp rise is seen.

Figures 3 and 4 are spectral emissivities for liquid platinum and liquid gold, respectively, as a function of temperature at the four wavelengths studied. The spectral emissivities of liquid platinum and gold show a moderate temperature dependence at all the wavelengths. The results of a least squares fit $E_\lambda = a + bT$ are tabulated on the plot. In the case of liquid platinum, the data at 514.5nm shows substantial curvature but no higher order fits were attempted. Moderate temperature dependencies of the spectral emissivities were also observed for Ni, Pd, Cu, Ag, and Zr at the four wavelengths studied.

Two important results reported here are the observations that (1) the spectral emissivities at the four wavelengths of the metals in the Ni and Cu groups show moderate temperature dependencies over the temperature ranges studied and (2) the spectral emissivities of the liquids are *higher* than those of the corresponding solids. Furthermore, in those liquid metals were moderate supercooling was observed, the measured spectral emissivities of the supercooled liquid were essentially the same as those of the liquid above the melting point.

To demonstrate the large increases in emissivities on melting of metals, measurements of the spectral emissivities of solid copper and palladium were performed just below their melting point by allowing them to freeze within the levitation coil. The emissivity measured for solid copper was 0.10, while the palladium the value was 0.32 (for the He-Ne wavelength). These are 15-20% lower than the emissivities of the corresponding liquids. A similar increase of about 13% was observed in the green for palladium. Intuitively, one expects the smoother, liquid surface, to have a lower emissivity than the solid. This would be the case if the only factors affecting emissivity were macroscopic physical and chemical structures of the surface; however, the optical properties are also governed by the electronic properties. Simple expansion on melting would alter the band structure. Furthermore, the lack of an ordered structure in the liquid (although short range order may be present) may provide at least part of the basis for the changes observed in the optical properties upon melting of these metals.

Comparison of the dielectric functions and complex index of refraction data with those available in the literature[14-15,17] showed excellent agreement for the low melting materials. There are no previous data for liquid Pd, Pt, and Zr.

This work has been supported by the National Aeronautics and Space Administration and by the U. S. Department of Energy through a contract with E. I. Du Pont de Nemours, Inc., at the Savannah River Laboratory.

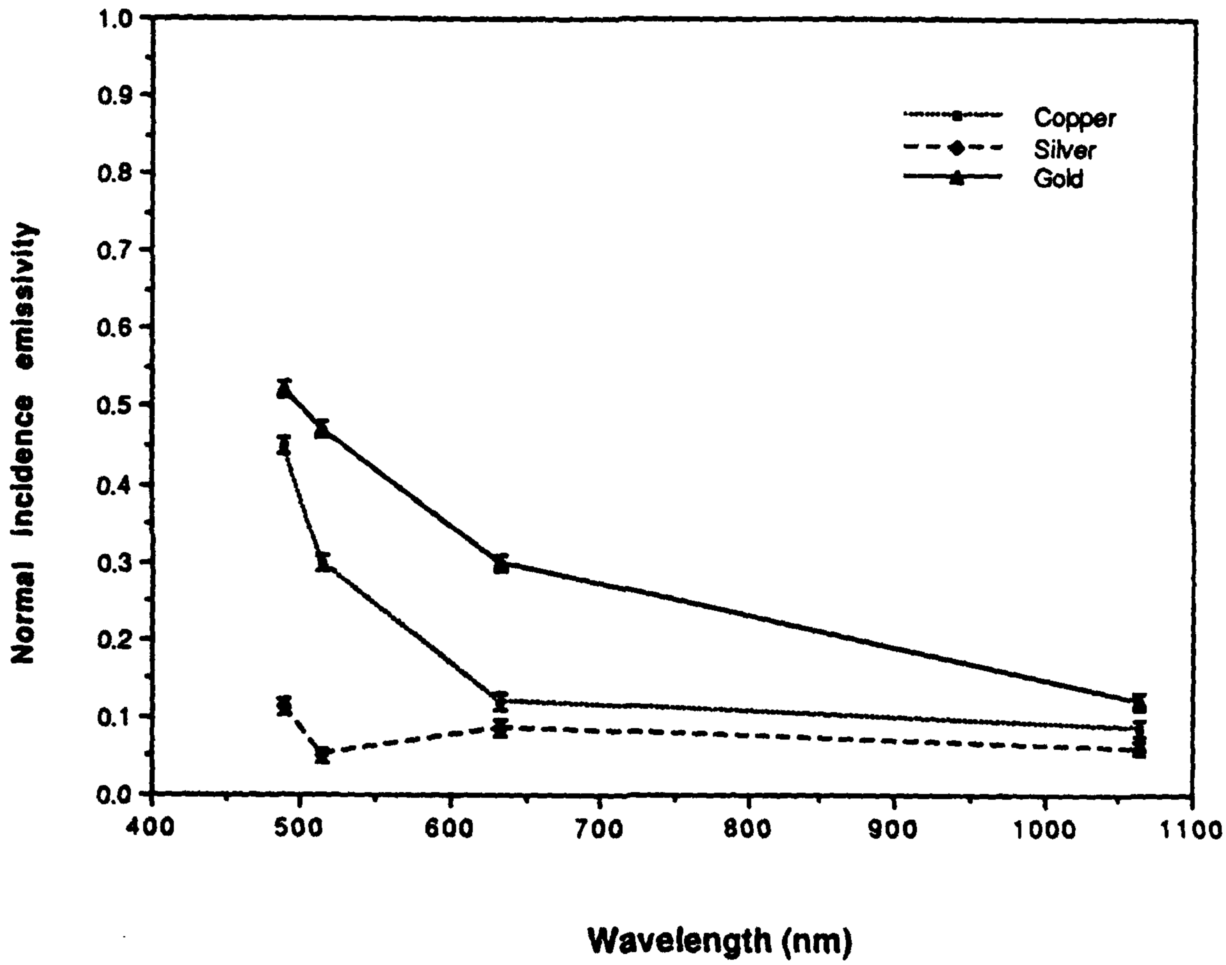

Figure 1. Spectral emissivities of liquid copper, silver and gold at various wave lengths.

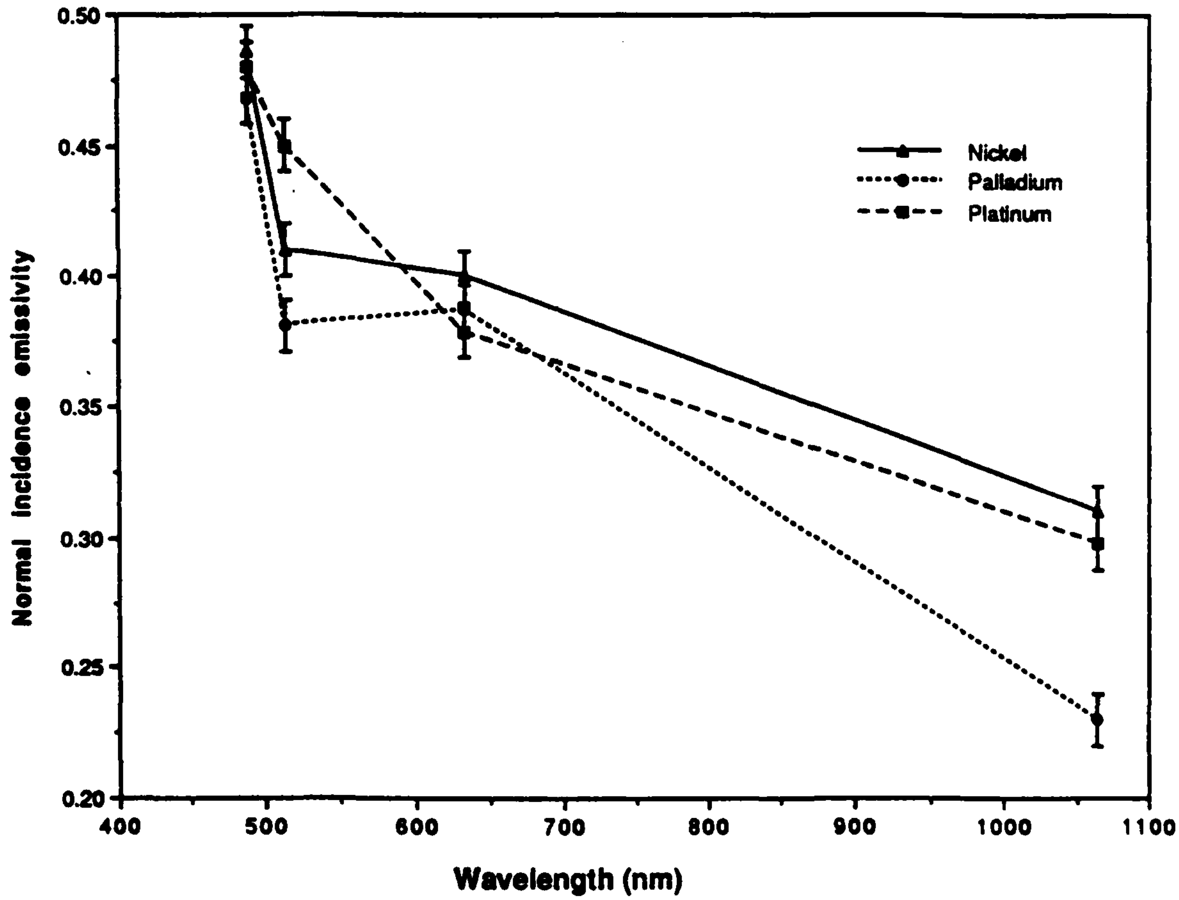

Figure 2. Spectral emissivities of liquid nickel, palladium and platinum at various wave lengths.

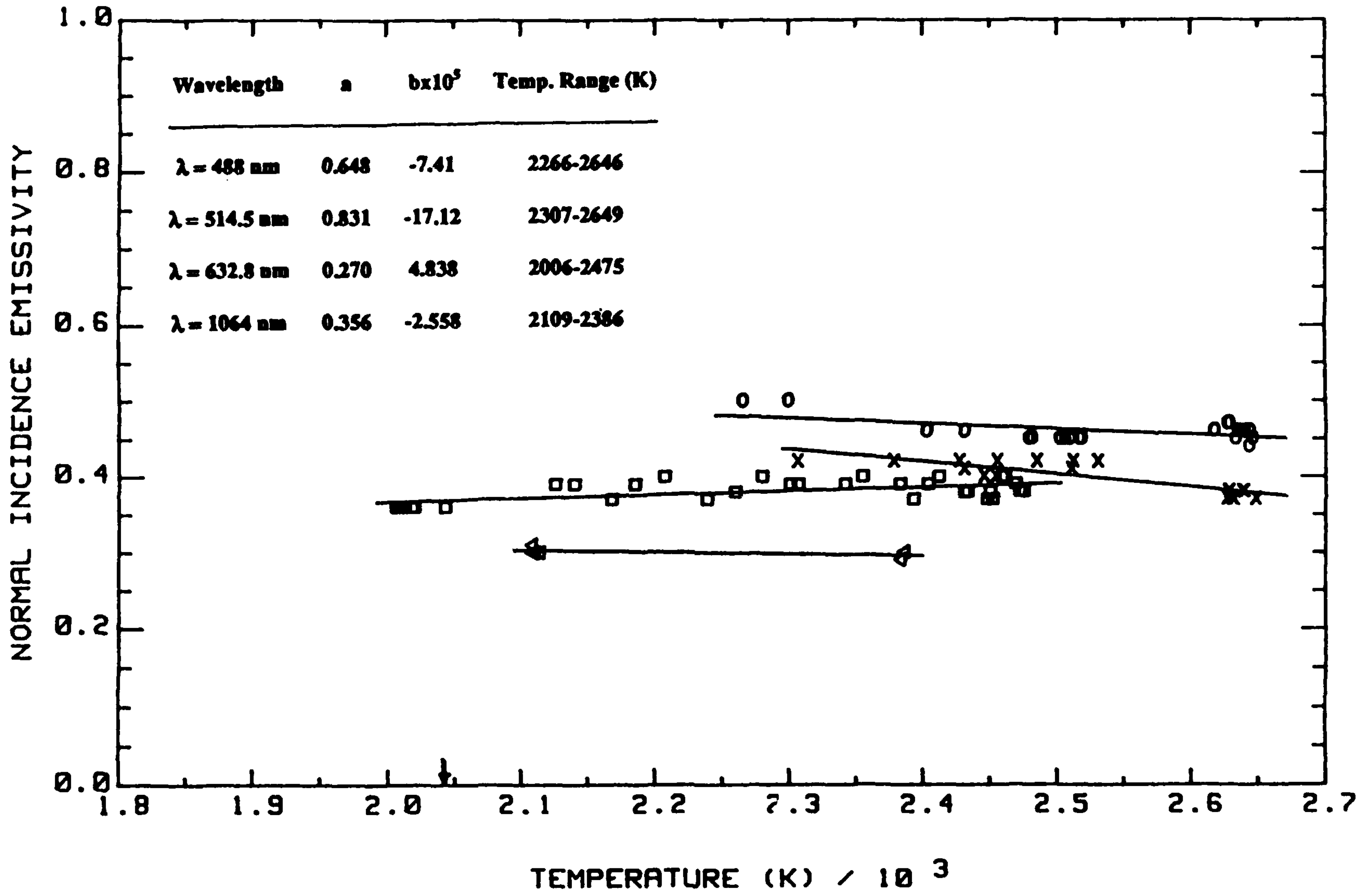

Figure 3. Spectral emissivities of liquid platinum at 448, 514.5, 632.8 and 1064nm at various temperatures.

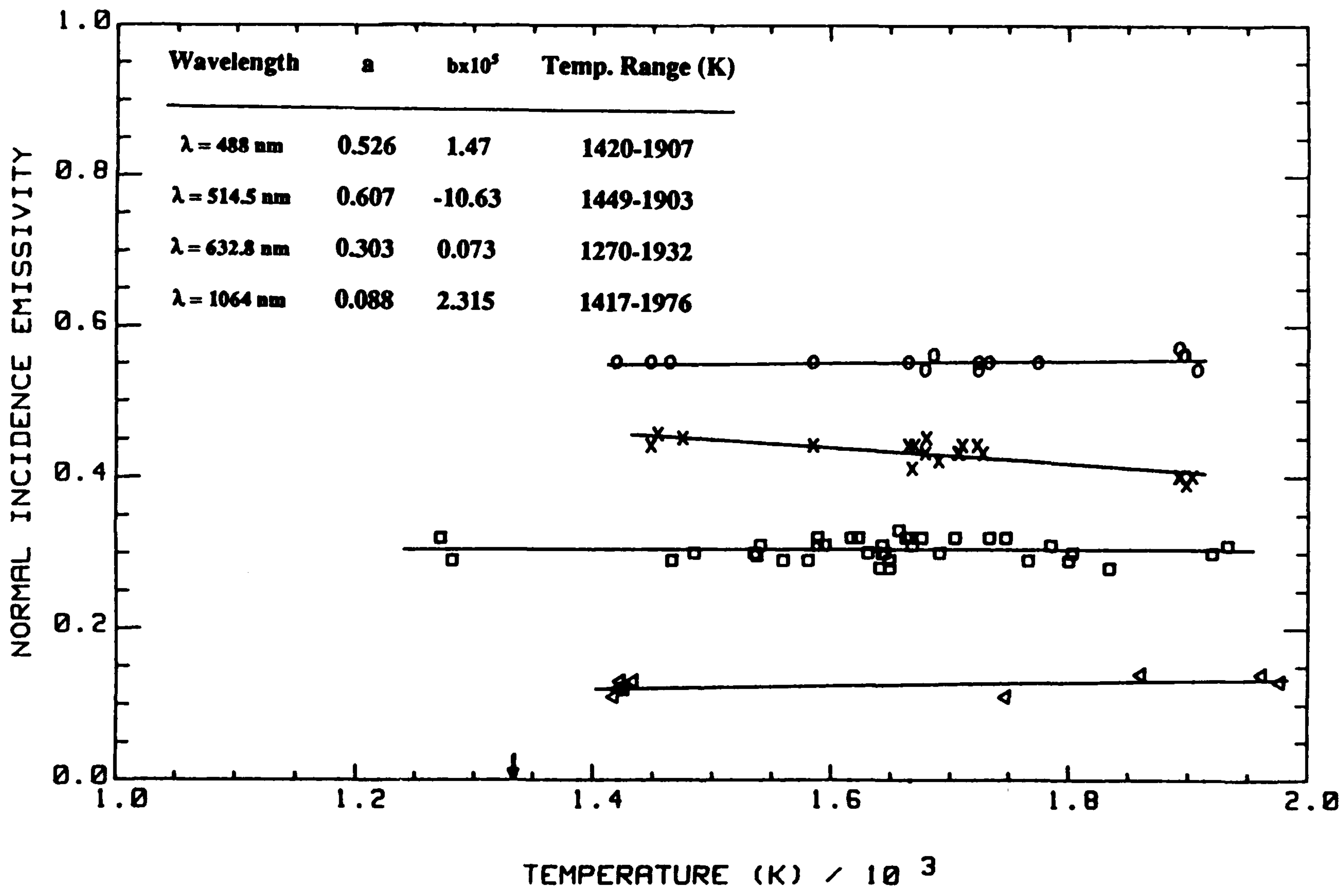

Figure 4. Spectral emissivities of liquid gold at 488, 514.5, 632.8 and 1064nm at various temperatures.

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ADVANCED SYSTEMS FOR ADSORPTION OF TOXIC GASES

J. Economy

INTRODUCTION

Activated carbons (charcoal) have found extensive use for protection of military personnel against toxic gases. For example, they are used routinely in masks for infantry and filters for tanks. Such assemblies have been used for over 50 years with little change and have proven to be reasonably reliable. One variation introduced during World War II was the incorporation of chromium into the carbon (Whetlarized) to provide a mechanism for decomposing gases such as cyanogen chloride.

Today, with increasing sophistication in the design of toxic gases (nerve gases); potential for terrorist attacks on seemingly unprotectable military structures including water supply, and possibility for wide spread use in third world countries to control restive populaces, there appears to be a need to design and develop far more versatile systems for protection which address these needs. In addition, there are several critical limitations with the current systems that require immediate attention. These include:

1. No mechanism for reactivation of spent carbons in the field.
2. No method to measure useful life in the field.
3. Disposal of Whetlarized carbons creates a major pollution problem by contaminating ground water with chromium.
4. Contact efficiency for removing highly toxic gases below several ppm drops off sharply.

Finally, there is little or no fundamental understanding on a) the mechanisms of adsorption operation in activated carbons b) the processes

involved in controlling pore diameter and its distribution during activation and c) low temperature mechanisms for reactivating surfaces. Clearly any meaningful progress in designing advanced systems for chemical protection must be accompanied by a much better understanding of the fundamental underpinnings of this technology.

DISCUSSION

It is useful to briefly review the nature of the activated carbon systems now in use. Because of their granular or particulate nature they require encapsulation in relatively bulky containers. The mechanism for activation involves heating carbons at high temperature of 800°-1000°C in the presence of gases such as steam to yield very high surface areas of at least 1000 m^2/g. Because of impurities and inhomogeneities in the carbons a range of pore diameters from 3-4Å up to 20-50Å are formed in this process. The larger pores act as transitional pores providing more direct contact with the environment while the finer pores provide the more effective adsorption capability. Typically the carbonaceous surface in these pores is highly oxidized and probably consists of carboxylic acids, phenolic hydroxyls and quinone units. Such surfaces should be effective in adsorbing a wide range of polar and non-polar molecules because of hydrogen bonding, acid base interactions, dipolar interactions and Van der Waals forces all operative within these very small pores. Because of the relatively acidic nature of the surface one would expect a significant discrimination in adsorptivity with basic gases being strongly bonded and more acidic gases being more easily displaced presumably with much higher transport characteristics. With such knowledge one could imagine designing mixtures of gases where the toxic component has the highest

transport characteristics and thus has the potential to defeat the protection system. For example, in actual field use the activated carbon in gas masks may become saturated with exhaust from tanks and thus permit more acidic toxic gases to easily pass through the carbon. It should also be noted that because of the particulate nature of the granules the contact efficiency may drop off sharply below a few ppm. This problem can be further exacerbated by settling in the cannister which can provide open pathways for penetration of toxic gases.

One approach that could address practically all of the problems enumerated above would be through the use of activated carbon fibers. Such fibers were first developed by the PI about 20 years ago and were made available in limited commercial quantities by the Carborundum Co. and its licenser, Nippon Kynol. From this work a number of key observations were made that would suggest solutions to most all of the above problems. These include the following:

1. High surface area carbon fibers (2000 m^2/g) can be made in a wide range of highly durable textile forms including fabrics, felt, paper, etc. (Available today from Nippon Kynol Co. in Japan.)

2. The fibers can be prepared by activating phenolic fiber precursors (Kynol) to achieve pores with either acidic or basic surfaces depending on the environment for activation.

3. The activated carbon fibers display a small but uniform pore diameter distribution with no transitional pores, which increases the breakthrough time by 40%. The interstitial openings between fibers act to fill the role of the transitional pores. The carbon surfaces in these textiles have been shown to be

more effective than granules in removing trace contaminant, down in the ppb range.

4. The fabrics can be reactivated to recover 100% of the original activity by in situ electrical resistance heating of the fibers to ~200°C, thus making such systems extremely cost effective.

5. It was observed that one could air activate much lower cost organic fibers at temperatures of 300-400°C to achieve high surface area adsorption characteristics similar to the carbons.

6. The micropores in the activated carbon fibers were shown to form a continuous network (based on density measurements) suggesting possible design of molecular filters consisting of an activated carbon film supported on a porous ceramic hollow tube.

Of the above indicated observations the last five are of a very preliminary nature growing out of earlier studies of the author.

For key to a successful program on design of advanced chemical systems for personnel protection it essential that a broad SED st''dy aimed at greatly upgrading the fundamental understanding of activated carbons also be pursued. Questions that must be addressed include:

a. What are the key structural features in the precursor materials which control pore volume and distribution, carbon yield, etc.? With this knowledge one may be able to design improved, lower cost precursor materials for use in design of activated carbon assemblies.

b. what are the mechanisms operative in etching of carbons to achieve surface areas of at least 2000 m^2/g and yet permit preservation of the fibrous shape of the precursor? Besides the traditional approaches based on steam or CO_2 activation are there alternative approaches such as lower temperature

plasma techniques which would yield high surface area fibers in much higher yield with uniquely tailored surfaces? Are these concepts extendable to a much wider range of organic fibers besides the phenolic precursor?

c. How are materials adsorbed on the activated surfaces? Use of advanced surface analysis techniques such as time of flight SIMS and ESCA should provide direct information on the nature of surface interactions and also on the number of layers of molecules held securely on the surface. Such studies would also elucidate the role of the pore diameter in tailoring activated carbons for use in liquid vs. gas adsorption.

d. Fundamental understanding of adsorption/desorption kinetics are essential in terms of designing systems which will desorb at very low temperatures of 100-200°C. Are there other concepts that one could conceive of to effectively desorb gases other than thermal?